

A POSTERIORI ERROR ESTIMATES FOR ENERGY-BASED QUASICONTINUUM APPROXIMATIONS OF A PERIODIC CHAIN

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ABSTRACT. We present a posteriori error estimates for a recently developed atomistic/continuum coupling method, the Consistent Energy-Based QC Coupling method. The error estimate of the deformation gradient combines a residual estimate and an a posteriori stability analysis. The residual is decomposed into the residual due to the approximation of the stored energy and that due to the approximation of the external force, and are bounded in negative Sobolev norms. In addition, the error estimate of the total energy using the error estimate of the deformation gradient is also presented. Finally, numerical experiments are provided to illustrate our analysis.

1. INTRODUCTION

Quasicontinuum (QC) methods, or in general atomistic/continuum coupling methods, are a class of multiscale methods for coupling an atomistic model of a solid with a continuum model. These methods have been widely employed in computational nano-technology, where a fully atomistic model will result in a prohibitive computational cost but an exact configuration is required in a certain region of the material. In this situation, atomistic model is applied in the region which contains the defect core to retain certain accuracy, while continuum model is applied in the far field to reduce the computational cost.

A number of QC methods have been developed in the past decades and are classified in two groups: energy-based coupling methods and force-based coupling methods. Despite the fact that the force-based methods are easy to implement and extend to higher dimensional cases, energy-based methods have certain advantages. For example, the forces derived from an energy potential are conservative which could leads to a faster convergence rate in computation, and the energy of an atomistic system can also be a quantity of interest in real application. However, consistent energy-based coupling methods can be tedious and restrictive on the shape of the coupling interface in more than one dimension (see [11, 4]) and it was not until recent that a practical consistent energy-based coupling method was created by Shapeev [10], which is the Consistent Energy-Based QC Coupling method that we analyze in the present paper.

A number of literature on the rigorous analysis of different QC methods have been proposed since the first one by Lin [5]. However, most of the analysis are on the a priori error analysis, and only a few are on the a posteriori error analysis. Arndt and Luskin give a posteriori error estimates for the QC approximation of a Frenkel-Kontorova model [2, 3, 1]. A goal-oriented approach is used and error estimates on different quantity of interests, each of which is essentially the difference between the values of a linear functional at the atomistic solution and the QC solution, are proposed. The estimates are decomposed into two parts, one is used to correctly chose the atomistic region and another is used to optimally choose the mesh in the continuum region. Serge et al. [9] give error estimates, also through a goal-oriented approach, of the original energy-based QC approximation, whose consistency is not guaranteed. Both

of the above works employ the technique of deriving and solving dual problems as a result of the goal-oriented approach. Ortner and Süli [7] derive an a posteriori error indicator for a global norm through a similar approach as ours. However, the QC method analyzed there does not contain an approximation of the stored energy which is essentially different from the QC method we are interested.

The present paper provides the a posteriori error analysis for the Consistent Energy-Based QC Coupling method [10] for a one dimensional periodic chain with nearest and next nearest neighbour interactions. The formulation of the QC approximation has the feature that the finite element nodes in the continuum region are not restricted to reside at the atomistic positions, which creates the situation that interaction bonds often cross the element boundaries, which is common in two dimensional formulation. We then derive the residual in negative Sobolev norms and then the a posteriori stability constant as a function of the QC solution. The error estimator of the deformation gradient in L_2 -norm is then obtained by combining these two analysis. In addition, we derive an error estimator for the total energy difference by using that of the deformation gradient. It should be remarked that though both of the error estimators are global quantities, they consist of contributions from element. As a result, an adaptive mesh refinement algorithm is developed and applied to a problem that mimics the vacancy in the two dimensional case, and the numerical results are presented.

1.1. Outline. In Section 2, we first formulate the atomistic model through both a continuous approach, i.e., the deformation and the displacement are considered as continuous functions on the reference lattice, and a discrete approach, which is always taken in previous literature. We then formulate the Consistent Energy-Based QC Coupling method in one dimensional setting.

In Section 3, we derive the residual estimates for the Consistent Energy-Based QC Coupling method in a negative Sobolev norm. The residual is split into two part, one is due to the approximation of the stored energy and the other is due to the approximation of the external force.

In Section 4, we give the a posteriori stability analysis.

In Section 5, we combine the residual estimate and the stability analysis to give the a posteriori error estimate of the deformation gradient in L_2 -norm and that of the total energy.

In Section 6, we present a numerical example to complement our analysis.

2. MODEL PROBLEM AND QC APPROXIMATION

2.1. Atomistic Model. As opposed to taking only a discrete point of view in many QC researches, we use both continuous functions and discretized vectors to denote the displacement and the deformation. The reason for doing this is that the Consistent Energy-Based QC coupling method, which we analyze in this paper, is easily formulated through the continuous approach, while discrete formulations could make the residual analysis of the external forces much easier.

For an infinite reference lattice with atomistic spacing ε , we make the partition $\mathcal{T}^\varepsilon = \{T_\ell^\varepsilon\}_{\ell=-\infty}^\infty$ of the domain \mathbb{R} such that $\mathbb{R} = \cup_{\ell=-\infty}^\infty T_\ell^\varepsilon$ and $T_\ell^\varepsilon = [(\ell-1)\varepsilon, \ell\varepsilon]$. We then define the displacement and deformation of this infinite lattice to be continuous piecewise linear functions $u, y \in \mathcal{P}_1(\mathcal{T}^\varepsilon) \cap C^0(\mathbb{R})$. We use \mathbf{u} and \mathbf{y} to denote the vectorizations of u and y such that $u_\ell = u(\ell\varepsilon)$ and $y_\ell = y(\ell\varepsilon)$. We know that u_ℓ and y_ℓ are the physical displacement and deformation of atom ℓ respectively.

To avoid technical difficulties with boundaries, we apply periodic boundary conditions. We rescale the problem so that there are $N \in \mathbb{N}$ atoms in each period and $\varepsilon = 1/N$, which implies that u and y are 1-periodic functions and \mathbf{u} and \mathbf{y} are N -periodic vectors. We also impose a

zero-mean condition to the admissible space of displacements, which is defined to be

$$\mathcal{U} = \left\{ u \in \mathcal{P}_1(\mathcal{T}^\varepsilon) \cap C^0(\mathbb{R}) : u(x+1) = u(x) \text{ and } \int_0^1 u(x) dx = 0 \right\}. \quad (2.1)$$

The set of admissible deformations is given by

$$\mathcal{Y} = \left\{ y \in \mathcal{P}_1(\mathcal{T}^\varepsilon) \cap C^0(\mathbb{R}) : y(x) = Fx + u(x), u \in \mathcal{U} \right\}, \quad (2.2)$$

where $F > 0$ is a given macroscopic deformation gradient.

As we mentioned above, it is necessary in the analysis of the external forces to employ the discretization of the displacement and the deformation. Therefore, by the relationship between u, y and their vectorizations \mathbf{u}, \mathbf{y} , the discrete space of displacement and the admissible set of deformation are defined by

$$\mathcal{U}^\varepsilon = \left\{ \mathbf{u} \in \mathbb{R}^{\mathbb{Z}} : u_{\ell+N} = u_\ell, \varepsilon \sum_{\ell=1}^N u_\ell = 0 \right\}, \quad (2.3)$$

and

$$\mathcal{Y}^\varepsilon = \left\{ \mathbf{y} \in \mathbb{R}^{\mathbb{Z}} : y_{\ell+N} = F\varepsilon + u_\ell, \mathbf{u} \in \mathcal{U}^\varepsilon \right\}, \quad (2.4)$$

where the zero-mean condition on the displacements, i.e., $\varepsilon \sum_{\ell=1}^N u_\ell = 0$ is obtained by applying the trapezoidal rule to evaluate the integration $\int_0^1 u(x) dx$ with respect to the partition \mathcal{T}^ε and using the periodicity of u .

For simplicity of analysis, we adopt a pair interaction model and assume that only nearest neighbours and the next-nearest neighbours interact. With a slight abuse of notation, the *stored atomistic energy* (per period) of an admissible deformation is then given by

$$\begin{aligned} \mathcal{E}_a(y) &:= \varepsilon \sum_{\ell=1}^N \phi\left(\frac{y(\ell\varepsilon) - y((\ell-1)\varepsilon)}{\varepsilon}\right) + \varepsilon \sum_{\ell=1}^N \phi\left(\frac{y(\ell\varepsilon) - y((\ell-2)\varepsilon)}{\varepsilon}\right) \\ &= \varepsilon \sum_{\ell=1}^N \phi\left(\frac{y_\ell - y_{\ell-1}}{\varepsilon}\right) + \varepsilon \sum_{\ell=1}^N \phi\left(\frac{y_\ell - y_{\ell-2}}{\varepsilon}\right) =: \mathcal{E}_a(\mathbf{y}), \end{aligned} \quad (2.5)$$

where $\phi \in C^3((0, +\infty))$ is a Lennard-Jones type interaction potential. We assume that there exists $r_* > 0$ such that ϕ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$.

For the formulation of the external energy, we first define the linear nodal interpolation operator $I_\varepsilon : C^0(\mathbb{R}) \rightarrow \mathcal{P}_1(\mathcal{T}^\varepsilon) \cap C^0(\mathbb{R})$ such that

$$I_\varepsilon g(\ell\varepsilon) = g(\ell\varepsilon) \quad \forall g \in C^0(\mathbb{R}). \quad (2.6)$$

Then given a dead load $f \in \mathcal{U}$, we define the *external energy* (per period) caused by f to be

$$\langle f, u \rangle_\varepsilon := \int_0^1 I_\varepsilon(fu) dx = \sum_{\ell=1}^N \varepsilon f_\ell u_\ell =: \langle \mathbf{f}, \mathbf{u} \rangle_\varepsilon, \quad (2.7)$$

where \mathbf{f} and \mathbf{u} are the vectorizations of the external force f and the displacement u according to \mathcal{T}^ε .

Thus, the *total energy* (per period) under a deformation $y \in \mathcal{Y}$ is given by

$$E_a(y; F) = \mathcal{E}_a(y) - \langle f, u \rangle_\varepsilon,$$

as u is determined by y and F . However, in our analysis, we always assume that F is given and as a result, we simply write $E_a(y; F)$ as $E_a(y)$.

The problem we wish to solve is to find

$$y_a \in \operatorname{argmin} E_a(\mathcal{Y}), \quad (2.8)$$

where argmin denotes the set of local minimizers.

2.2. Notation of Partitions, Norms and Discrete Derivatives. Though it is natural to introduce the QC approximation after the atomistic model, we decide to pause here and introduce some important notation that are used throughout the paper in order to make the flow of the paper more smooth and save some space.

In Section 2.1, we have introduced the partition \mathcal{T}^ε of the domain \mathbb{R} . We now fix the notation for a generalized partition.

Let $\mathcal{T}^m = \{T_k^m\}_{k=-\infty}^\infty$ be a given partition such that $T_k^m = [x_{k-1}^m, x_k^m]$, where $x_k^m > x_{k-1}^m$ are the nodes of the partition. We denote the size (or the length) of the k 'th element by $\varepsilon_k^m := |T_k^m| = x_k^m - x_{k-1}^m$. We also define the mesh size vector $\boldsymbol{\varepsilon}^m$ such that $\boldsymbol{\varepsilon}^m := (\varepsilon_k^m)_{k=-\infty}^\infty \in (\mathbb{R}^+)^{\mathbb{Z}}$.

Given a partition \mathcal{T}^m and a function $g \in C^0(\mathbb{R})$, we define the \mathcal{P}_1 direct interpolation $I_m : C^0(\mathbb{R}) \rightarrow \mathcal{P}_1(\mathcal{T}^m) \cap C^0(\mathbb{R})$ by

$$(I_m g)(x_i^m) = g(x_i^m) \quad \forall g \in C^0(\mathbb{R}), \quad (2.9)$$

and $I_m g$ is often denoted by g_m . We also denote the vectorization of $g \in C^0(\mathbb{R})$ with respect to \mathcal{T}^m by \mathbf{g}^m such that

$$g_j^m = g(x_j^m). \quad (2.10)$$

Let \mathcal{D} be a subset of \mathbb{Z} . For a vector $\mathbf{v} \in \mathbb{R}^{\mathbb{Z}}$ and a partition \mathcal{T}^m , we define the (semi-)norms

$$\|\mathbf{v}\|_{\ell_{\boldsymbol{\varepsilon}^m}^p(\mathcal{D})} = \begin{cases} \left(\sum_{\ell \in \mathcal{D}} \varepsilon_\ell^m |v_\ell|^p \right)^{1/p}, & 1 \leq p < \infty, \\ \max_{\ell \in \mathcal{D}} |v_\ell|, & p = \infty. \end{cases}$$

In particular, if n_m is the number of the nodes of \mathcal{T}^m that are in $[0, 1]$, we simply define

$$\|\mathbf{v}\|_{\ell_{\boldsymbol{\varepsilon}^m}^p} = \begin{cases} \left(\sum_{\ell=1}^{n_m} \varepsilon_\ell^m |v_\ell|^p \right)^{1/p}, & 1 \leq p < \infty, \\ \max_{\ell=1, \dots, n_m} |v_\ell|, & p = \infty. \end{cases}$$

We now define discrete derivatives. Suppose $v \in C^0(\mathbb{R})$ and \mathbf{v}^m is its vectorization according to \mathcal{T}^m . We define the first and second order discrete derivative $\mathbf{v}^{m'}$ by

$$v_k^{m'} = \frac{v_j^m - v_{j-1}^m}{\varepsilon_j^m}, \text{ and } v_k^{m''} = \frac{v_{j+1}^{m'} - v_j^{m'}}{\bar{\varepsilon}_j^m}, \quad (2.11)$$

where $\bar{\varepsilon}_j^m := \frac{1}{2}(\varepsilon_j^m + \varepsilon_{j+1}^m)$.

It can be proved that for $v^m \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^m)$ and \mathbf{v}^m being its vectorization, we have the identity

$$\|v^{m'}\|_{L^p[0,1]} = \|\mathbf{v}^{m'}\|_{\ell_{\boldsymbol{\varepsilon}^m}^p}. \quad (2.12)$$

Since \mathcal{T}^ε is special and uniform, we simply use $\boldsymbol{\varepsilon}$ and ε to denote its mesh size vector and mesh size without superscripts and subscripts.

In addition to these, we denote the left and the right limit of an open interval ω by L_ω and R_ω , which are also used later in our analysis.

2.3. QC Approximation. The QC approximation we analyze in this paper is essentially the Consistent Atomistic/Continuum Coupling method developed in [10]. We briefly redevelop this method in 1D so that it is easily understood and enough for us to carry out the analysis.

We first decompose the reference lattice, which occupies \mathbb{R} , into an atomistic region Ω_a , which should contain any 'defects', and a continuum region Ω_c , where the solution is expected to be smooth. Moreover, we assume Ω_a to be a union of open intervals and Ω_c to be a union of closed intervals, and $\Omega_a \cup \Omega_c = \mathbb{R}$. Since we impose periodic boundary conditions on the displacement and notationally it is easier to assume the atomistic region is away from the boundary of the period we analyze, we make the following assumptions on Ω_a and Ω_c :

- Ω_a and Ω_c appear periodically with exactly period of 1, i.e, if $x \in \Omega_a$ then $x + 1 \in \Omega_a$ and the same for Ω_c .
- $\exists \delta > 2\varepsilon$ such that $((0, \delta) \cup (1 - \delta, 1)) \subset \Omega_c$, i.e., the atomistic region is contained in the 'middle' of the chain.

Note that, there is no such a restriction, that the interfaces where different regions meet should lie on the positions of the atoms, i.e., it is not necessary that $\Omega_c \cap \Omega_a \in \varepsilon\mathbb{Z}$, which was always assumed in previous modeling and analysis of 1D QC method.

Then, in order to reduce the number of degrees of freedom, we make the partition $\mathcal{T}^h = \{T_k^h\}_{k=-\infty}^{\infty}$ of the domain \mathbb{R} according to the above region decomposition of \mathbb{R} as follows:

- $T_k^h = [x_k^h, x_{k-1}^h]$ and $T_{k+K} = [x_k^h + 1, x_{k-1}^h + 1] = [x_{k+K}^h, x_{k-1+K}^h]$, which implies that the partition is K -periodic with $|\cup_{k=1}^K T_k| = 1$, and there are K elements in each $[0, 1]$. We also assume that x_1^h is the left most node and x_K^h is the right most node in $[0, 1]$.
- If $\ell\varepsilon \in \Omega_a$, then $\exists i \in \mathbb{Z}$ such that $x_i = \ell\varepsilon$, i.e., every position of an atom in the atomistic region is a node of this partition.
- $\partial\Omega_c$ is a node in this partition which means that each element is contained in only one of the two regions.
- $|T_k^h| = \varepsilon_k^h \geq 2\varepsilon$ if $T_k^h \subset \Omega_c$, i.e., the size of each element in the continuum region is larger than or equal to 2ε .

We emphasize two definitions

$$\ell_k := \max_{\ell} \{\ell : \ell\varepsilon \leq x_k^h\} \text{ and } \theta_k := \frac{x_k^h - \ell_k\varepsilon}{\varepsilon}, \quad (2.13)$$

which are extensively used in the analysis and significantly simplify the notation. Note that $0 \leq \theta_k \leq 1$.

Based on this partition of the domain, the QC space of displacement and the QC set of admissible deformation are defined by

$$\mathcal{U}_{\text{qc}} = \left\{ u \in \mathcal{P}_1(\mathcal{T}^h) \cap C^0(\mathbb{R}) : u(x+1) = u(x) \text{ and } \int_0^1 u(x) dx = 0 \right\}, \quad (2.14)$$

and

$$\mathcal{Y}_{\text{qc}} = \left\{ y \in \mathcal{P}_1(\mathcal{T}^h) \cap C^0(\mathbb{R}) : y(x) = Fx + u(x), u \in \mathcal{U}_{\text{qc}} \right\}. \quad (2.15)$$

The discrete QC space of displacement and the QC set of admissible deformation are defined by

$$\mathcal{U}_{\text{qc}}^h = \left\{ \mathbf{u}^h \in \mathbb{R}^{\mathbb{Z}} : u_k^h = u_{k+K}^h, \forall k \in \mathbb{Z}, \text{ and } \sum_{k=1}^K \frac{1}{2} (x_{k+1}^h - x_{k-1}^h) u_k^h = 0 \right\}, \quad (2.16)$$

and

$$\mathcal{Y}_{\text{qc}}^h = \left\{ \mathbf{y}^h \in \mathbb{R}^{\mathbb{Z}} : y_k^h = Fx_k + u_k^h, \mathbf{u} \in \mathcal{U}_{\text{qc}}^h \right\}. \quad (2.17)$$

Note that unlike \mathcal{U}^ε and \mathcal{Y}^ε , in which every vector has the physical displacements and deformations of the atoms as its components, \mathcal{U}^h and \mathcal{Y}^h only contain vectors whose components are the values of displacements and deformations at the nodes of \mathcal{T}^h .

The approach to couple the atomistic and continuum energy is to associate the energy with interaction bonds. The term *bond* between atoms $i \in \mathbb{Z}$ and $i + r \in \mathbb{Z}$ refer to the open interval $b = (i\varepsilon, (i + r)\varepsilon)$. In our case, since only nearest neighbour and next nearest neighbour bonds are taken into account, $r = 1, 2$ only.

To develop the coupling method, we define the operator $D_\omega y$ for an open interval $\omega = (L_\omega, R_\omega) \subset \mathbb{R}$ and $y \in C^0(\mathbb{R})$ such that

$$D_\omega y := \frac{1}{|\omega|} (y(R_\omega) - y(L_\omega)). \quad (2.18)$$

If we take any $y \in C^0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ as a deformation (note that this 'deformation' might be non-physical) and a bond $b = (i\varepsilon, (i + r_b)\varepsilon)$, we can define the atomistic energy contribution of bond b to the stored energy to be

$$a_b(y) = \frac{|b \cap \Omega_a|}{r_b} \phi(r_b D_{b \cap \Omega_a} y), \quad (2.19)$$

and its continuum energy contribution to the stored energy to be

$$c_b(y) = \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx, \quad (2.20)$$

where $\nabla_{r_b} y = r_b y'(x)$.

Since we are only interested in the situation in $[0, 1]$, which is extended periodically to the whole domain, the set of bonds that we will consider is

$$\mathcal{B} = \{(i\varepsilon, (i + r)\varepsilon) : r = 1, 2, i = 0, 1, \dots, N - 1\}. \quad (2.21)$$

Therefore, coupling the two energy contributions together, the *stored QC energy* (per period) of a deformation $y \in C^0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ is then given by

$$\mathcal{E}_{\text{qc}}(y) = \sum_{b \in \mathcal{B}} [a_b(y) + c_b(y)], \quad (2.22)$$

which was shown in [10] to be a consistent coupling method, where the definition of consistency is as follows:

$$\mathcal{E}'_a(Fx)[v] = \mathcal{E}'_{\text{qc}}(Fx)[v] = 0 \quad \forall v \in C^0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R}). \quad (2.23)$$

Given a dead load $f \in \mathcal{U}$ the QC approximation of the *external energy* (per period) caused by f is given by

$$\langle f, u_h \rangle_h := \int_0^1 I_h(f u_h) \, dx = \sum_{k=1}^K \frac{1}{2} (x_{k+1}^h - x_{k-1}^h) f_k^h u_k^h =: \langle \mathbf{f}^h, \mathbf{u}^h \rangle_h, \quad (2.24)$$

where I_h is the linear nodal interpolation with respect to \mathcal{T}^h , and \mathbf{f}^h and \mathbf{u}^h are the vectorizations of f and u_h .

Thus, the *total energy* (per period) of a deformation $y_h \in \mathcal{Y}_{\text{qc}}$ is given by

$$E_{\text{qc}}(y_h; F) = \mathcal{E}_{\text{qc}}(y_h) - \langle f, u_h \rangle_h.$$

For the same reason that F is given, we write $E_{\text{qc}}(y_h; F)$ as $E_{\text{qc}}(y_h)$. The problem we wish to solve is to find

$$y_{\text{qc}} \in \operatorname{argmin} E_{\text{qc}}(\mathcal{Y}_{\text{qc}}). \quad (2.25)$$

3. RESIDUAL ANALYSIS

In this section, we bound the residual in a negative Sobolev norms. We equip the space \mathcal{U} with the Sobolev norm

$$\|v\|_{\mathcal{U}^{1,2}} = \|v'\|_{L^2[0,1]}, \quad \text{for } v \in \mathcal{U},$$

and denote it by $\mathcal{U}^{1,2}$. The norm on the dual $\mathcal{U}^{-1,2} := (\mathcal{U}^{1,2})^*$ is defined by

$$\|T\|_{\mathcal{U}^{-1,2}} := \sup_{\substack{v \in \mathcal{U} \\ \|v\|_{\mathcal{U}^{1,2}}=1}} T[v], \quad \text{for } T \in \mathcal{U}^{-1,2}.$$

In the following sections, we formulate the problems in variational forms and then analyze the residual.

3.1. Variational Formulation and Residual. Let y_a be a solution of the atomistic problem (2.8). If $y_a'(x) > 0$ on $[0, 1]$, $\mathcal{E}_a(y)$ has the variational derivative at y_a and therefore, the first order optimality condition for (2.8) in variational form is

$$\mathcal{E}'_a(y_a)[v] = \langle f, v \rangle_\varepsilon \quad \forall v \in \mathcal{U}, \quad (3.1)$$

where

$$\mathcal{E}'_a(y_a)[v] = \varepsilon \sum_{b \in \mathcal{B}} \phi'(r_b D_b y_a) r_b D_b v. \quad (3.2)$$

Let y_{qc} be a solution of the QC problem (2.25). If $y_{qc}'(x) > 0$ on $[0, 1]$, then $\mathcal{E}_{qc}(y)$ has the variational derivative at y_{qc} and the first order optimality condition for (2.25) in variational form is

$$\mathcal{E}'_{qc}(y_{qc})[v_h] = \langle f, v_h \rangle_h \quad \forall v_h \in \mathcal{U}_{qc}, \quad (3.3)$$

where

$$\begin{aligned} \mathcal{E}'_{qc}(y_h)[v_h] &= \sum_{b \in \mathcal{B}} [a'_b(y_h)[v_h] + c_b(y_h)[v_h]] \\ &= |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v_h + \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v_h \, dx \quad \forall v_h \in \mathcal{U}_{qc}. \end{aligned} \quad (3.4)$$

In conforming finite element analysis, where the finite element solution space is a subspace of the original solution space, the residual is defined as the quantity we obtain by inserting the computed solution to the equation which the real solution satisfies. However, in our case, \mathcal{Y}_{qc} is in general not a subspace of \mathcal{Y}_a , and hence the functional $\mathcal{E}_a(\cdot)$ is not defined on \mathcal{Y}_{qc} in general and $\mathcal{E}_{qc}(\cdot)$ is not defined on \mathcal{Y}_a either. The way through which we circumvent this difficulty is to define mappings between the solution spaces so that the residual could be well defined. In concrete, we define $J_{\mathcal{U}} : \mathcal{U} \rightarrow \mathcal{U}_{qc}$ and $J_{\mathcal{U}_{qc}} : \mathcal{U}_{qc} \rightarrow \mathcal{U}$ such that

$$J_{\mathcal{U}} u = I_h u - \frac{1}{2} \sum_{\ell=1}^K (x_{k+1}^h - x_{k-1}^h) u(x_k^h) \quad \forall u \in \mathcal{U}, \quad (3.5)$$

and

$$J_{\mathcal{U}_{qc}} u_h = I_\varepsilon u_h - \varepsilon \sum_{\ell=1}^N u_h(\ell \varepsilon) \quad \forall u_h \in \mathcal{U}_{qc}. \quad (3.6)$$

It is easy to check that $J_{\mathcal{U}}u$ and $J_{\mathcal{U}_{\text{qc}}}u_h$ satisfy the corresponding mean zero condition of \mathcal{U} and \mathcal{U}_{qc} , which implies that $J_{\mathcal{U}}u \in \mathcal{U}_{\text{qc}}$ and $J_{\mathcal{U}_{\text{qc}}}u_h \in \mathcal{U}$. With a slight abuse of notation, we define

$$J_{\mathcal{U}}y = Fx + J_{\mathcal{U}}u = Fx + I_h u - \frac{1}{2} \sum_{\ell=1}^K (x_{k+1}^h - x_{k-1}^h) u(x_k^h) = I_h y - \frac{1}{2} \sum_{\ell=1}^K (x_{k+1}^h - x_{k-1}^h) u(x_k^h) \quad \forall y \in \mathcal{U}, \quad (3.7)$$

and

$$J_{\mathcal{U}_{\text{qc}}}y_h = Fx + J_{\mathcal{U}_{\text{qc}}}u_h = Fx + I_{\varepsilon} u_h - \frac{1}{2} \varepsilon \sum_{\ell=1}^N u_h(\ell \varepsilon) = I_{\varepsilon} y - \frac{1}{2} \varepsilon \sum_{\ell=1}^N u_h(\ell \varepsilon) \quad \forall y_h \in \mathcal{U}_{\text{qc}}. \quad (3.8)$$

We then define the residual (at the solution y_{qc}) to be

$$\begin{aligned} R[v] &= E'_a(J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}})[v] \\ &= E'_a(J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}})[v] - E'_{\text{qc}}(y_{\text{qc}})[v] \\ &= [\mathcal{E}'_a(J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}})[v] - \langle f, v \rangle_{\varepsilon}] - [\mathcal{E}'_{\text{qc}}(y_{\text{qc}})[J_{\mathcal{U}}v] - \langle f, J_{\mathcal{U}}v \rangle_h] \\ &= [\mathcal{E}'_a(J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}})[v] - \mathcal{E}'_{\text{qc}}(y_{\text{qc}})[J_{\mathcal{U}}v]] + [\langle f, J_{\mathcal{U}}v \rangle_h - \langle f, v \rangle_{\varepsilon}]. \end{aligned} \quad (3.9)$$

and understand R as a functional in $\mathcal{U}^{-1,2}$. By this formulation, we essentially split the residual into two parts: the first part is the residual of the stored energy and the second part is the residual of the external force. We will bound these two parts in the following sections.

3.2. Estimate of the Residual of the Stored Energy. In this section, we analyze the first part of (3.9), which is the residual of the stored energy.

Before we give the theorem, we make several definitions that simplify our notation.

First, we define the set \mathcal{K}_c to be

$$\mathcal{K}_c := \{k : k \in \{1, \dots, K\} \text{ such that } T_k \cap [0, 1] \neq \emptyset \text{ but } T_k \cap (1, +\infty) = \emptyset \text{ and } T_k \subset \Omega_c\}, \quad (3.10)$$

which is essentially the set of indices of the elements in the continuum region in $[0, 1]$.

Second, suppose the atomistic region consists of M disjoint subregions in $[0, 1]$, i.e., $\Omega_a \cap [0, 1] = \cup_{i=1}^M \Omega_a^i$ among which $\Omega_a^i \cap \Omega_a^j = \emptyset$ if $i \neq j$, we define the nodes lie on the atomistic-continuum interface of the atomistic regions be $x_{La_i}^h$, $i = 1, \dots, M$ and those lie on the right interface be $x_{Rc_i}^h$, $i = 1, \dots, M$.

Third, we define $\mathcal{K}'_c \subset \mathcal{K}_c$ to be the set of indices of the elements in the continuum region but not adjacent to an atomistic region, i.e., $\forall k \in \mathcal{K}'_c$, $k \neq La_i$ and $k - 1 \neq R_{a_i}$, $\forall i \in \{1, 2, \dots, M\}$.

Using these definitions, we have the following theorem.

Theorem 1. For $y_h \in \mathcal{Y}$ with $y'_h(x) > 0$, we have

$$\|\mathcal{E}'_a(J_{\mathcal{U}_{\text{qc}}}y_h)[\cdot] - \mathcal{E}'_{\text{qc}}(y_h)[J_{\mathcal{U}}\cdot]\|_{\mathcal{U}^{-1,2}} \leq \left\{ \sum_{k \in \mathcal{K}_c} \eta_k^{e2} \right\}^{\frac{1}{2}} =: \mathcal{E}_{\text{store}}(y_h), \quad (3.11)$$

where

$$\eta_k^e = \left(\frac{1}{2} \sum_{j=0}^2 [[\phi']]_{\ell_{k-1}+j}^2 + \frac{1}{2} \sum_{j=0}^2 [[\phi']]_{\ell_k+j}^2 \right)^{\frac{1}{2}}, \quad (3.12)$$

if $k \in \mathcal{K}'_c$,

$$\eta_k^e = \left(\varepsilon \sum_{j=0}^2 [[\phi']]_{\ell_{La_i}+j}^2 + \frac{1}{2} \varepsilon \sum_{j=0}^2 [[\phi']]_{\ell_{k-1}+j}^2 \right)^{\frac{1}{2}}, \quad (3.13)$$

if $k = L_{a_i}$ for some $i \in \{1, 2, \dots, M\}$, i.e., T_k is adjacent to and to the left of an atomistic region, and

$$\eta_k^\varepsilon = \left(\varepsilon \sum_{j=0}^2 [[\phi']]_{\ell_{Ra_i+j}}^2 + \frac{1}{2} \varepsilon \sum_{j=0}^2 [[\phi']]_{\ell_{k+j}}^2 \right)^{\frac{1}{2}}, \quad (3.14)$$

if $k-1 = R_{a_i}$ for some $i \in \{1, 2, \dots, M\}$, i.e., T_k is adjacent to and to the right of an atomistic region. $[[\phi']]_\ell$'s will be defined in the proof.

Proof. By (3.2) and (3.4), we have

$$\begin{aligned} \mathcal{E}'_a(J_{\mathcal{U}_{qc}} y_h)[v] - \mathcal{E}'_{qc}(y_h)[J_{\mathcal{U}} v] &= \varepsilon \sum_{b \in \mathcal{B}} \phi'(r_b D_b J_{\mathcal{U}_{qc}} y_h) r_b D_b v - \sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} J_{\mathcal{U}} v \\ &\quad - \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} J_{\mathcal{U}} v \, dx \\ &= \varepsilon \sum_{b \in \mathcal{B}} \phi'(r_b D_b y_h) r_b D_b v - \sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} I_h v \\ &\quad - \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} I_h v \, dx, \end{aligned} \quad (3.15)$$

since $D_b J_{\mathcal{U}_{qc}} y_h = D_b I_\varepsilon y_h = D_b y_h$, $D_\omega J_{\mathcal{U}} v = D_\omega I_h v$ for any ω being an open interval, and $(J_{\mathcal{U}} v)' = (I_h v)'$, which can be easily verified by noting that $J_{\mathcal{U}_{qc}} y_h$ and $J_{\mathcal{U}} v$ are $I_\varepsilon y_h$ and $I_h v$ shifted by some constants.

To make further analysis of (3.15), we subtract and add the same terms

$$\sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v \text{ and } \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx$$

to get

$$\begin{aligned} \mathcal{E}'_a(J_{\mathcal{U}_{qc}} y_h)[v] - \mathcal{E}'_{qc}(y_h)[J_{\mathcal{U}} v] &= \sum_{b \in \mathcal{B}} \left\{ \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v \right. \\ &\quad \left. - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \right\} \\ &\quad - \left\{ \sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) [D_{b \cap \Omega_a} I_h v \, dx - D_{b \cap \Omega_a} v] \right\} \\ &\quad - \left\{ \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) [\nabla_{r_b} I_h v - \nabla_{r_b} v] \, dx \right\}. \end{aligned} \quad (3.16)$$

We first analyze the second and third groups, which turn out to be 0 as we will see immediately.

For the second group, we have,

$$\begin{aligned} &\sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) [D_{b \cap \Omega_a} I_h v \, dx - D_{b \cap \Omega_a} v] \\ &= \sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) \left[\frac{I_h v(R_{b \cap \Omega_a}) - I_h v(L_{b \cap \Omega_a})}{R_{b \cap \Omega_a} - L_{b \cap \Omega_a}} - \frac{v(R_{b \cap \Omega_a}) - v(L_{b \cap \Omega_a})}{R_{b \cap \Omega_a} - L_{b \cap \Omega_a}} \right]. \end{aligned} \quad (3.17)$$

We define the above to be 0 if $b \cap \Omega_a = \emptyset$. If $b \cap \Omega_a \neq \emptyset$, since both $R_{b \cap \Omega_a}$ and $L_{b \cap \Omega_c}$ are either at atomistic positions in Ω_a or on $\partial\Omega_c$, they must be nodes in \mathcal{T}^h . Therefore, by the definition of $I_h v$, the following holds

$$I_h v(L_{b \cap \Omega_a}) = v(L_{b \cap \Omega_a}) \text{ and } I_h v(R_{b \cap \Omega_a}) = v(R_{b \cap \Omega_a}),$$

which implies that (3.17) is 0.

For the third group, upon defining $\chi_{\mathcal{S}}$ to be the characteristic function of a set \mathcal{S} , we can rewrite it as

$$\begin{aligned} & \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) [\nabla_{r_b} I_h v - \nabla_{r_b} v] \, dx \\ &= \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{\Omega_c} \chi_b \phi'(\nabla_{r_b} y_h) [\nabla_{r_b} I_h v - \nabla_{r_b} v] \, dx \\ &= \sum_{b \in \mathcal{B}} \frac{1}{r_b} \sum_{k \in \mathcal{K}_c} \int_{T_k} \chi_b \phi'(\nabla_{r_b} y_h) [\nabla_{r_b} I_h v - \nabla_{r_b} v] \, dx \\ &= \sum_{r=1}^2 \sum_{b \in \mathcal{B}, r_b=r} \sum_{k \in \mathcal{K}_c} \frac{1}{r_b} \int_{T_k} \chi_b \phi'(\nabla_{r_b} y_h) [\nabla_{r_b} I_h v - \nabla_{r_b} v] \, dx \\ &= \sum_{r=1}^2 \sum_{k \in \mathcal{K}_c} \sum_{b \in \mathcal{B}, r_b=r} \frac{1}{r_b} \int_{T_k} \chi_b \phi'(\nabla_r y_h) [\nabla_r I_h v - \nabla_r v] \, dx \\ &= \sum_{r=1}^2 \sum_{k \in \mathcal{K}_c} \phi'(\nabla_r y_h|_{T_k}) \int_{T_k} \left[\sum_{b \in \mathcal{B}, r_b=r} \frac{1}{r_b} \chi_b \right] [\nabla_r I_h v - \nabla_r v], \end{aligned} \quad (3.18)$$

since $\nabla_r y_h|_{T_k}$ is a constant on each element. By the 1D bond density lemma[10, Lemma 3.4],

$$\sum_{b \in \mathcal{B}, r_b=r} \frac{1}{r} \chi_b(x) =_{a.e.} 1,$$

we have

$$\begin{aligned} & \sum_{r=1}^2 \sum_{k \in \mathcal{K}_c} \phi'(\nabla_r y_h|_{T_k}) \int_{T_k} \left[\sum_{b \in \mathcal{B}, r_b=r} \frac{1}{r_b} \chi_b \right] [\nabla_r I_h v - \nabla_r v] \\ &= \sum_{r=1}^2 \sum_{k \in \mathcal{K}_c} \phi'(\nabla_{r_b} y_h|_{T_k}) \left[r(I_h v(x_k) - I_h v(x_{k-1})) - r(v(x_k) - v(x_{k-1})) \right]. \end{aligned} \quad (3.19)$$

Again by the definition of $I_h v$,

$$I_h v(x_k^h) = v(x_k^h) \text{ and } I_h v(x_{k-1}^h) = v(x_{k-1}^h),$$

and thus (3.19) is 0.

Now we turn to the analysis of the first group and analyze

$$\varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \quad (3.20)$$

for each interaction bond b .

If $b \subset \Omega_a$, we have $|b \cap \Omega_c| = r_b \varepsilon$, $|b \cap \Omega_a| = 0$ and the equivalence of the operators $D_b = D_{b \cap \Omega_a}$. We know that (3.20) is 0 by substituting these equivalences.

If $b \subset \Omega_c \cap T_k$ for some $k \in \mathcal{K}_c$, then $|b \cap \Omega_c| = r_b \varepsilon$ and $|b \cap \Omega_a| = 0$. We also note that $\nabla_{r_b} y_h(x) = r_b D_b y_h$, as y_h is affine on T_k , and $\frac{1}{r_b} \int_{b \cap \Omega_c} \nabla_{r_b} v = \varepsilon r_b D_b v$. Using these equivalences, we know that (3.20) is again 0.

Therefore, we only need to analyze the bonds crossing the atomistic-continuum interface or the boundaries of two adjacent elements in Ω_c . Because of its tediousness, we leave the detailed analysis to the Appendix but just present the result here. Employing the notation often adopted by a posteriori error analysis for elliptic equations, we have the following result

$$\begin{aligned}
 & \varepsilon \sum_{b \in \mathcal{B}} \phi'(r_b D_b I_\varepsilon y_h) r_b D_b v - \sum_{b \in \mathcal{B}} |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v + \sum_{b \in \mathcal{B}} \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\
 &= \sum_{i=1}^M \varepsilon \left\{ [[\phi']]_{\ell_{La_i}} v'_{\ell_{La_i}} + [[\phi']]_{\ell_{La_i}+1} v'_{\ell_{La_i}+1} + [[\phi']]_{\ell_{La_i}+2} v'_{\ell_{La_i}+2} \right\} \\
 &+ \sum_{i=1}^M \varepsilon \left\{ [[\phi']]_{\ell_{Ra_i}} v'_{\ell_{Ra_i}} + [[\phi']]_{\ell_{Ra_i}+1} v'_{\ell_{Ra_i}+1} + [[\phi']]_{\ell_{Ra_i}+2} v'_{\ell_{Ra_i}+2} \right\} \\
 &+ \sum_{k \in \mathcal{K}'_c} \varepsilon \left\{ [[\phi']]_{\ell_k} v'_{\ell_k} + [[\phi']]_{\ell_k+1} v'_{\ell_k+1} + [[\phi']]_{\ell_k+2} v'_{\ell_k+2} \right\}, \tag{3.21}
 \end{aligned}$$

where for $k = La_i$,

$$[[\phi']]_\ell = \phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - \phi'(2 y'_h|_{T_k}), \tag{3.22}$$

$$\begin{aligned}
 [[\phi']]_{\ell+1} &= \left[\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) - \theta_k \phi'(y'_h|_{T_k}) \right] \\
 &+ \left[(1 - \theta_k) \phi'\left(\frac{2}{2 - \theta_k} y'_h|_{T_{k+2}} + \frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}}\right) \right. \\
 &\quad \left. + \theta_k \phi'(2 y'_h|_{T_k}) - \phi'(y'_h|_{T_{k+2}} + (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) \right] \\
 &+ \left[(1 - \theta_k) \phi'(2 y'_h|_{T_{k+1}}) + \theta_k \phi'(2 y'_h|_{T_k}) - \phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) \right] \tag{3.23}
 \end{aligned}$$

$$[[\phi']]_{\ell+2} = \phi'\left(\frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}} + \frac{2}{2 - \theta_k} y'_h|_{T_{k+2}}\right) - \phi'(y'_h|_{T_{k+2}} + (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}), \tag{3.24}$$

for $k = Ra_i$

$$[[\phi']]_\ell = \phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) - \phi'\left(\frac{2\theta_k}{(1 + \theta_k)} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}\right), \tag{3.25}$$

$$\begin{aligned}
[[\phi']]_{\ell+1} = & \left[\theta_k \phi'(y'_h|_{T_k}) + (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) - \phi'((1 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) \right] \\
& + \left[\theta_k \phi' \left(\frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}} \right) + (1 - \theta_k) \phi'(2y'_h|_{T_{k+1}}) \right. \\
& \left. - \phi'((1 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) \right] \\
& + \left[(1 - \theta_k) \phi'(2y'_h|_{T_{k+1}}) + \theta_k \phi'(2y'_h|_{T_k}) - \phi'((2 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) \right] \quad (3.26)
\end{aligned}$$

$$[[\phi']]_{\ell+2} = \phi'(2y'_h|_{T_{k+1}}) - \phi'((2 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}), \quad (3.27)$$

and for $k \in \mathcal{K}'_c$

$$[[\phi']]_{\ell} = \phi'(2y'_h|_{T_k}) - \phi'((1 - \theta_k)y'_h|_{T_{k+1}} + (1 + \theta_k)y'_h|_{T_k}), \quad (3.28)$$

$$\begin{aligned}
[[\phi']]_{\ell+1} = & \left[(1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) + \theta_k \phi'(y'_h|_{T_k}) - \phi'((1 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) \right] \\
& + \left[2(1 - \theta_k) \phi'(2y'_h|_{T_{k+1}}) + 2\theta_k \phi'(2y'_h|_{T_k}) \right. \\
& \left. - \phi'((2 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \phi'((1 - \theta_k)y'_h|_{T_{k+1}} + (1 + \theta_k)y'_h|_{T_k}) \right], \quad (3.29)
\end{aligned}$$

$$[[\phi']]_{\ell+2} = \phi'(2y'_h|_{T_{k+1}}) - \phi'((2 - \theta_k)y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}). \quad (3.30)$$

Distributing the contribution of (3.21) to each element and applying Cauchy-Schwarz inequality, we obtain the estimate stated in the theorem. \square

3.3. Estimate of the Residual of the External Force. We now turn to the estimate of the residual of the external energy. Upon defining $J_{\mathcal{U}}v := v_h$, the residual of the external force is given by

$$\langle f, v_h \rangle_h - \langle f, v \rangle_{\varepsilon}, \quad (3.31)$$

where $f, v \in \mathcal{U}$.

To further analyze (3.31), we introduce a new partition $\mathcal{T}^r = \{T_j^r\}_{j=-\infty}^{+\infty}$ of the domain \mathbb{R} , such that all the nodes in partition $\mathcal{T}^{\varepsilon}$ and partition \mathcal{T}^h are included in this partition. The indexing of the nodes in \mathcal{T}^r follow the rule that the node x_k^h in \mathcal{T}^h is labeled as $x_{j_k}^r$ in \mathcal{T}^r . We also assume there are n nodes in \mathcal{T}^r in $[0, 1]$, i.e.,

$$n = |\{\varepsilon, 2\varepsilon, \dots, N\varepsilon\} \cup \{x_1, x_2, \dots, x_K\}|,$$

where $|\mathcal{A}|$ denote the cardinality of a finite set \mathcal{A} .

The inner product associated with \mathcal{T}^r partition is then defined by

$$\langle f, g \rangle_r := \int_0^1 I_r(fg) dx = \sum_{j=1}^n \frac{1}{2} (x_{j+1}^r - x_{j-1}^r) f_j^r g_j^r =: \langle \mathbf{f}^r, \mathbf{g}^r \rangle_r \quad \forall f, g \in C^0(\mathbb{R}), \quad (3.32)$$

where I_r is the linear nodal interpolation operator with respect to \mathcal{T}^r , and \mathbf{f}^r and \mathbf{g}^r are the vectorizations of f and g with respect to \mathcal{T}^r .

Now we decompose the residual of the external force into three parts by adding and subtracting the same terms,

$$\langle f, v_h \rangle_h - \langle f, v \rangle_{\varepsilon} = [\langle f, v \rangle_r - \langle f, v \rangle_{\varepsilon}] + [\langle f, v_h \rangle_r - \langle f, v \rangle_r] + [\langle f, v_h \rangle_h - \langle f, v_h \rangle_r]. \quad (3.33)$$

The following three lemma are derived to give the estimates of the three parts.

Lemma 2. *Let $\mathbf{f}, \mathbf{v}, \mathbf{f}^r, \mathbf{v}^r$ be the vectorizations of $f, v \in C^0(\mathbb{R})$ according to \mathcal{T}^ε and \mathcal{T}^r . Then the following inequality holds*

$$|\langle f, v \rangle_r - \langle f, v \rangle_\varepsilon| = |\langle \mathbf{f}^r, \mathbf{v}^r \rangle_r - \langle \mathbf{f}, \mathbf{v} \rangle_\varepsilon| \leq \frac{1}{8} \varepsilon^2 \|\mathbf{f}'\|_{\ell_\varepsilon^2(\mathcal{K}_U)} \|\mathbf{v}'\|_{\ell_\varepsilon^2}, \quad (3.34)$$

where $\mathcal{K}_U = \{k \in \{1, \dots, K\} : x_k \neq \ell_k \varepsilon\}$, in other words, \mathcal{K}_U is the set of indices of the nodes x_k^h in \mathcal{T}^h such that x_k^h does not coincide with any of the nodes in \mathcal{T}^ε .

Proof. We first write out the two inner products and eliminate the terms that are the same

$$\begin{aligned} \langle \mathbf{f}^r, \mathbf{v}^r \rangle_r - \langle \mathbf{f}, \mathbf{v} \rangle_\varepsilon &= \sum_{\ell=1}^n \varepsilon_\ell^r \frac{1}{2} (f_\ell^r v_\ell^r + f_{\ell+1}^r v_{\ell+1}^r) - \sum_{\ell=1}^N \varepsilon \frac{1}{2} (f_\ell v_\ell + f_{\ell+1} v_{\ell+1}) \\ &= \sum_{k \in \mathcal{K}_U} \left(\varepsilon_{j_k} \frac{1}{2} (f_{j_k-1}^r v_{j_k-1}^r + f_{j_k}^r v_{j_k}^r) + \varepsilon_{j_k+1} \frac{1}{2} (f_{j_k}^r v_{j_k}^r + f_{j_k+1}^r v_{j_k+1}^r) \right) \\ &\quad - \sum_{k \in \mathcal{K}_U} \varepsilon (f_{\ell_k} v_{\ell_k} + f_{\ell_k+1} v_{\ell_k+1}), \end{aligned} \quad (3.35)$$

as $\varepsilon_{j_k+2} = \varepsilon_{j_k+3} = \dots = \varepsilon_{j_{k+1}-1} = \varepsilon$ and $f_{\ell_k+i} v_{\ell_k+i} = f_{j_k+i}^r v_{j_k+i}^r$, $i = 1, 2, \dots, \ell_{k+1} - \ell_k$, if $\ell_k \varepsilon \neq x_k$ and $\ell_{k+1} \varepsilon \neq x_{k+1}$.

For k such that $\ell_k \varepsilon \neq x_k$, by the definition of $\mathbf{f}, \mathbf{v}, \mathbf{f}^r$ and \mathbf{v}^r , we have $f_{\ell_k} = f_{j_k-1}^r$, $v_{\ell_k} = v_{j_k-1}^r$, $f_{\ell_k+1} = f_{j_k+1}^r$ and $v_{\ell_k+1} = v_{j_k+1}^r$. We also have $f_{j_k}^r = (1 - \theta_k) f_{\ell_k} + \theta_k f_{\ell_k+1}$ and $v_{j_k}^r = (1 - \theta_k) v_{\ell_k} + \theta_k v_{\ell_k+1}$. Inserting these equalities, (3.35) can be estimated as

$$\begin{aligned} &|\langle \mathbf{f}^r, \mathbf{v}^r \rangle_r - \langle \mathbf{f}, \mathbf{v} \rangle_\varepsilon| \\ &= \left| \sum_{k \in \mathcal{K}_U} \left\{ \frac{1}{2} \theta_k \varepsilon f_{\ell_k} v_{\ell_k} + \frac{1}{2} \theta_k \varepsilon [(1 - \theta_k) f_{\ell_k} + \theta_k f_{\ell_k+1}] [(1 - \theta_k) v_{\ell_k} + \theta_k v_{\ell_k+1}] \right. \right. \\ &\quad + \frac{1}{2} (1 - \theta_k) \varepsilon f_{\ell_k+1} v_{\ell_k+1} + \frac{1}{2} (1 - \theta_k) \varepsilon [(1 - \theta_k) f_{\ell_k} + \theta_k f_{\ell_k+1}] [(1 - \theta_k) v_{\ell_k} + \theta_k v_{\ell_k+1}] \\ &\quad \left. \left. - \frac{1}{2} \varepsilon f_{\ell_k} v_{\ell_k} - \frac{1}{2} \varepsilon f_{\ell_k+1} v_{\ell_k+1} \right\} \right| \\ &= \left| \sum_{k \in \mathcal{K}_U} \frac{1}{2} \varepsilon \left\{ [\theta_k (\theta_k - 1) (f_{\ell_k+1} - f_{\ell_k}) v_{\ell_k+1}] - [\theta_k (\theta_k - 1) (f_{\ell_k+1} - f_{\ell_k}) v_{\ell_k}] \right\} \right| \\ &= \sum_{k \in \mathcal{K}_U} \frac{1}{2} \varepsilon^3 |\theta_k (1 - \theta_k) f'_{\ell_k+1} v'_{\ell_k+1}| \\ &\leq \frac{1}{8} \varepsilon^2 \left(\sum_{k \in \mathcal{K}_U} \varepsilon |f'_{\ell_k+1}|^2 \right)^{\frac{1}{2}} \left(\sum_{k \in \mathcal{K}_U} \varepsilon |v'_{\ell_k+1}|^2 \right)^{\frac{1}{2}} \leq \frac{1}{8} \varepsilon^2 \|\mathbf{f}'\|_{\ell_\varepsilon^2(\mathcal{K}_U)} \|\mathbf{v}'\|_{\ell_\varepsilon^2}, \end{aligned} \quad (3.36)$$

which concludes the proof. \square

Remark 1. If $\mathcal{K} = \emptyset$, i.e., every node in \mathcal{T}^h is also in \mathcal{T}^ε , then this part of the residual is 0. \square

Lemma 3. *Let $f, v \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^\varepsilon)$ and $v_h = I_h v \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^h)$ be the \mathcal{P}_1 interpolation of v according to \mathcal{T}^h partition. Let $\mathbf{f}^r, \mathbf{v}^r$ and \mathbf{v}_h^r be the vectorizations of f, v, v_h respectively*

according to \mathcal{T}^r , and \mathcal{K}_c is defined in (3.10). Then we have the following estimate

$$\langle f, v_h \rangle_r - \langle f, v \rangle_r = \langle \mathbf{f}^r, \mathbf{v}_h^r \rangle_r - \langle \mathbf{f}^r, \mathbf{v}^r \rangle_r \leq \left[\sum_{k \in \mathcal{K}_c} \tilde{h}_k^2 \|\mathbf{f}^r\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^2)}^2 \right]^{\frac{1}{2}} \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}, \quad (3.37)$$

$\bar{\varepsilon}_j^r = \frac{1}{2}(\varepsilon_j^r + \varepsilon_{j+1}^r)$, $\tilde{h}_k = \frac{1}{2}(j_{k+1} - j_k)\varepsilon$ and $\mathcal{D}_k^2 = \{j_k + 1, \dots, j_{k+1} - 1\}$.

Proof. Using the fact that $(v_h^r)_{j_k} = v_{j_k}^r$ and by Cauchy-Schwarz inequality, we have

$$\begin{aligned} \langle \mathbf{f}^r, \mathbf{v}_h^r \rangle_r - \langle \mathbf{f}^r, \mathbf{v}^r \rangle_r &= \sum_{j=1}^n \frac{1}{2}(\varepsilon_j^r + \varepsilon_{j+1}^r)(f_j^r(v_h^r)_j - f_j^r v_j^r) \\ &= \sum_{k \in \mathcal{K}_c} \sum_{j=j_{k-1}}^{j_k-1} \bar{\varepsilon}_j^r f_j^r [(v_h^r)_j - v_j^r] \\ &\leq \sum_{k \in \mathcal{K}_c} \left[\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r (f_j^r)^2 \right]^{\frac{1}{2}} \left\{ \sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r [(v_h^r)_j - v_j^r]^2 \right\}^{\frac{1}{2}}, \end{aligned} \quad (3.38)$$

where $\bar{\varepsilon}_j^r = \frac{1}{2}(\varepsilon_j^r + \varepsilon_{j+1}^r)$. Upon defining \mathbf{g} such that $g_j = (v_h^r)_j - v_j^r$ (note $g_{j_k} = g_{j_{k+1}} = 0$) and by Lemma 15 in Appendix C (Discrete Friedrich's Inequality) and Rieze-Thorin Theorem,

$$\left\{ \sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r [(v_h^r)_j - v_j^r]^2 \right\}^{\frac{1}{2}} = \left\{ \sum_{j=j_{k-1}}^{j_k} \bar{\varepsilon}_j^r g_j^2 \right\}^{\frac{1}{2}} \leq \frac{1}{2}(j_k - j_{k-1})\varepsilon \left\{ \sum_{j=j_{k-1}+1}^{j_k} \varepsilon_j^r g_j'^2 \right\}^{\frac{1}{2}}, \quad (3.39)$$

where $g_j' = \frac{g_j - g_{j-1}}{\varepsilon_j^r} = (v_h^r)'_j - (v^r)'_j$. ε appears in the last inequality since $\max_j \bar{\varepsilon}_j^r \leq \varepsilon$. Since v_h^r and v^r are both piecewise linear on \mathcal{T}^r , we have $(v_h^r)'_j - (v^r)'_j = (v' - v_h')(x) \ \forall x \in (x_{j-1}^r, x_j^r)$, and as a result,

$$\left\{ \sum_{j=j_{k-1}+1}^{j_k} \varepsilon_j^r [(v_h^r)'_j - (v^r)'_j]^2 \right\}^{\frac{1}{2}} = \int_{x_{j_{k-1}}^r}^{x_{j_k}^r} |(v' - v_h')(x)|^2 dx = \|v' - v_h'\|_{L^2[x_{j_{k-1}}^r, x_{j_k}^r]}.$$

By Lemma 12 in Appendix B,

$$\|v' - v_h'\|_{L^2[x_{j_{k-1}}^r, x_{j_k}^r]} \leq \|v'\|_{L^2[x_{j_{k-1}}^r, x_{j_k}^r]}.$$

Put all the results above together and apply Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} &\sum_{k \in \mathcal{K}_c} \left[\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r (f_j^r)^2 \right]^{\frac{1}{2}} \left\{ \sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r [(v_h^r)_j - v_j^r]^2 \right\}^{\frac{1}{2}} \\ &\leq \sum_{k \in \mathcal{K}_c} \left\{ \tilde{h}_k \left(\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r f_j^{r2} \right)^{\frac{1}{2}} \|v'\|_{L^2(x_{j_{k-1}}^r, x_{j_k}^r)} \right\} \leq \left[\sum_{k \in \mathcal{K}_c} \tilde{h}_k^2 \left(\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r f_j^{r2} \right) \right]^{\frac{1}{2}} \|v'\|_{L^2[0,1]}. \end{aligned} \quad (3.40)$$

The estimate in the theorem holds as $\|v'\|_{L^2[0,1]} = \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}$ for $v \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^\varepsilon)$. \square

Lemma 4. Let $f, v \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^\varepsilon)$ and $v_h = I_h v \in C^0(\mathbb{R}) \cap \mathcal{P}_1(\mathcal{T}^h)$ be the \mathcal{P}_1 interpolation of v according to the \mathcal{T}^h . Let $\mathbf{f}^r, \mathbf{v}^r$ and \mathbf{v}_h^r be the vectorizations f, v and v_h according to \mathcal{T}^r .

If $\int_0^1 v_h = 0$, then we have the following estimate

$$\langle f, v_h \rangle_h - \langle f, v_h \rangle_r \leq \left\{ \frac{1}{8} \left[(n\varepsilon)^4 \sum_{k \in \mathcal{K}_c} \hat{h}_{k+1}^4 \|\mathbf{f}^{r''}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^2)}^2 \right]^{\frac{1}{2}} + \left[\sum_{k \in \mathcal{K}_c} \hat{h}_{k+1}^4 \|\mathbf{f}^{r'}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^1)}^2 \right]^{\frac{1}{2}} \right\} \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}. \quad (3.41)$$

where \mathcal{K}_c is defined in (3.10), $\mathcal{D}_k^1 = \{j_k + 1, \dots, j_{k+1}\}$ and \hat{h}_k will be defined in the proof.

Proof. Since $I_h(fv_h)$ is also piecewise linear with respect to the \mathcal{T}^r partition, we apply the trapezoidal rule here to evaluate $\langle f, v_h \rangle_h = \int_0^1 I_h(fv_h) dx$ to obtain

$$\begin{aligned} & \langle f, v_h \rangle_h - \langle f, v_h \rangle_r \\ &= \sum_{k \in \mathcal{K}_c} \left\{ \left[\frac{1}{2} \varepsilon_{j_{k-1}+1}^r I_h(fv_h)(x_k^r) + \sum_{j=j_{k-1}+1}^{j_k-1} \frac{1}{2} (\varepsilon_j^r + \varepsilon_{j+1}^r) I_h(fv_h)(x_j^r) + \frac{1}{2} \varepsilon_{j_k}^r I_h(fv_h)(x_{j_k}^r) \right] \right. \\ & \quad \left. - \left[\frac{1}{2} \varepsilon_{j_{k-1}+1}^r (fv_h)(x_{j_{k-1}+1}^r) + \sum_{j=j_{k-1}+1}^{j_k-1} \frac{1}{2} (\varepsilon_j^r + \varepsilon_{j+1}^r) (fv_h)(x_j^r) + \frac{1}{2} \varepsilon_{j_k}^r (fv_h)(x_{j_k}^r) \right] \right\}. \quad (3.42) \end{aligned}$$

We define \mathbf{g} and \mathbf{G} such that $g_j = (fv_h)(x_j^r)$ and $G_j = (I_h(fv_h))(x_j^r)$. It is easy to check that $g_{j_k} = G_{j_k}$ and

$$G_{j_{k-1}+i} = g_{j_{k-1}} + \frac{\sum_{\ell=1}^i \varepsilon_{j_{k-1}+\ell}^r}{\varepsilon_k^h} (g_{j_k} - g_{j_{k-1}}) \quad \forall k \in \mathcal{K}_c \quad \text{and} \quad i = 1, \dots, j_k - j_{k-1}, \quad (3.43)$$

where $\varepsilon_k^h = \sum_{j=j_{k-1}+1}^{j_k} \varepsilon_j^r = x_k - x_{k-1}$. Therefore, by Theorem 16, we obtain the following estimate

$$\begin{aligned} & |\langle f, v_h \rangle_h - \langle \mathbf{f}^r, I_r \mathbf{v}^h \rangle_r| \\ &= \left| \sum_{k \in \mathcal{K}_c} \left[\frac{1}{2} \varepsilon_{j_{k-1}}^r (g_{j_{k-1}} - G_{j_{k-1}}) + \sum_{j=j_{k-1}+1}^{j_k-1} \frac{1}{2} (\varepsilon_j^r + \varepsilon_{j+1}^r) (g_j - G_j) + \frac{1}{2} \varepsilon_{j_k}^r (g_{j_k} - G_{j_k}) \right] \right| \\ &\leq \sum_{k \in \mathcal{K}_c} \frac{1}{4} \frac{((j_k - j_{k-1})\varepsilon)((j_k - j_{k-1} + 1)\varepsilon)^2}{\varepsilon_k^h} \|\mathbf{g}''\|_{\ell_{\varepsilon^r}^1(\mathcal{D}_k^2)}, \quad (3.44) \end{aligned}$$

where \mathbf{g}'' is the second finite difference derivative with respect to the \mathcal{T}^r .

By the definition of \mathbf{f}^r and \mathbf{v}_h^r , $g_j = (fv_h)(x_j^r) = f_j^r(v_h^r)_j$. Using $(v_h^r)_j'' = 0 \quad \forall j \in \mathcal{D}_k^2$, g_j'' can be written as

$$g_j'' = (fv_h^r)_j'' = (f^r)_j''(v_h^r)_j + \frac{\varepsilon_j^r}{\varepsilon_j^r} (f^r)_j'(v_h^r)_j' + \frac{\varepsilon_{j+1}^r}{\varepsilon_j^r} (f^r)_{j+1}'(v_h^r)_{j+1}'. \quad (3.45)$$

Noting that $\frac{\varepsilon_j^r}{\bar{\varepsilon}_j} \leq 2$ and $\frac{\varepsilon_{j+1}^r}{\bar{\varepsilon}_j} \leq 2$ and defining $\hat{h}_k := \left[\frac{((j_k - j_{k-1})\varepsilon)(j_k - j_{k-1} + 1)\varepsilon}{\bar{\varepsilon}_k^n} \right]^{\frac{1}{2}}$, we have the following estimate

$$\begin{aligned}
\langle f, v_h \rangle_h - \langle f, v_h \rangle_r &\leq \sum_{k \in \mathcal{K}_c} \frac{1}{4} \hat{h}_k^2 \left[\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r |(f v_h'')_j| \right] \\
&\leq \sum_{k \in \mathcal{K}_c} \frac{1}{4} \hat{h}_k^2 \left[\sum_{j=j_{k-1}+1}^{j_k-1} \bar{\varepsilon}_j^r |(f^r)_j| |(v_h^r)_j| + 4 \sum_{j=j_{k-1}+1}^{j_k} \varepsilon_j^r |(f^r)_j| |(v_h^r)_j| \right] \\
&\leq \sum_{k \in \mathcal{K}_c} \frac{1}{4} \hat{h}_k^2 \left[\|\mathbf{f}^{r''}\|_{\ell_{\bar{\varepsilon}^r}^2(\mathcal{D}_k^2)} \|\mathbf{v}_h^r\|_{\ell_{\bar{\varepsilon}^r}^2(\mathcal{D}_k^2)} + 4 \|\mathbf{f}^{r'}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^1)} \|(\mathbf{v}_h^r)'\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^1)} \right] \\
&\leq \frac{1}{4} \left[\sum_{k \in \mathcal{K}_c} \hat{h}_k^4 \|\mathbf{f}^{r''}\|_{\ell_{\bar{\varepsilon}^r}^2(\mathcal{D}_k^2)}^2 \right]^{\frac{1}{2}} \|\mathbf{v}_h^r\|_{\ell_{\bar{\varepsilon}^r}^2} + \left[\sum_{k \in \mathcal{K}_c} \hat{h}_k^4 \|\mathbf{f}^{r'}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^1)}^2 \right]^{\frac{1}{2}} \|(\mathbf{v}_h^r)'\|_{\ell_{\varepsilon^r}^2}.
\end{aligned} \tag{3.46}$$

For further estimate, we first bound $\|\mathbf{v}_h^r\|_{\ell_{\bar{\varepsilon}^r}^2}$ by $\|(\mathbf{v}_h^r)'\|_{\ell_{\varepsilon^r}^2}$. Since $v_h(x)$ is piecewise linear with respect to \mathcal{T}^r partition, we can apply the trapezoidal rule to the integration on each element to get

$$\sum_{j=1}^n \bar{\varepsilon}_j^r (v_h^r)_j = \sum_{j=1}^n \frac{1}{2} (\varepsilon_j^r + \varepsilon_{j-1}^r) (v_h^r)_j = \sum_{j=1}^n \varepsilon_j^r \frac{1}{2} [(v_h^r)_j + (v_h^r)_{j+1}] = \int_0^1 v_h(x) dx = 0. \tag{3.47}$$

The last equality holds by the periodic condition on v_h . Thus, we can apply Lemma 14 in Appendix C and Riez-Thorin Theorem to obtain

$$\|\mathbf{v}_h^r\|_{\ell_{\bar{\varepsilon}^r}^2} \leq \frac{1}{2} n \varepsilon \left(\sum_{j=1}^n \varepsilon_j^r (v_h^r)_j'^2 \right)^{\frac{1}{2}}. \tag{3.48}$$

Since $v_h'(x) = (v_h^r)_j'$ on (x_{j-1}^r, x_j^r) ,

$$\sum_{j=1}^n \varepsilon_j^r (v_h^r)_j'^2 = \int_0^1 (v_h')^2 dx = \|v_h'\|_{L^2[0,1]}^2. \tag{3.49}$$

By Lemma 11 in Appendix B,

$$\|v_h'\|_{L^2[0,1]} \leq \|v'\|_{L^2[0,1]} = \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}. \tag{3.50}$$

Combine these results, the estimate stated in the theorem is easy to establish. \square

Having the three lemma and distribute the contribution to each element, we now give the theorem which essentially gives the estimate of the residual due to the external force.

Theorem 5. *For $f, v \in \mathcal{U}$ and $J_{\mathcal{U}}$ defined in (3.5), we have*

$$\|\langle f, J_{\mathcal{U}} \cdot \rangle_h - \langle f, \cdot \rangle_{\varepsilon}\|_{\mathcal{U}^{-1,2}} \leq \left\{ \sum_{k \in \mathcal{K}_c} \eta_k^{f^2} \right\}^{\frac{1}{2}} =: \mathcal{E}_{\text{ext}}(f), \tag{3.51}$$

where

$$\begin{aligned} \eta_k^f = & \left\{ \frac{1}{128} [\varepsilon^3 (f'_{\ell_{k-1}+1})^2 + \varepsilon^3 (f'_{\ell_k+1})^2]^2 + \tilde{h}_k^2 \|\mathbf{f}^r\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^2)}^2 \right. \\ & \left. + \frac{1}{64} (n\varepsilon)^4 \hat{h}_{k+1}^4 \|\mathbf{f}^{r''}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^2)}^2 + \hat{h}_{k+1}^4 \|\mathbf{f}^{r'}\|_{\ell_{\varepsilon^r}^2(\mathcal{D}_k^1)}^2 \right\}^{\frac{1}{2}}, \end{aligned} \quad (3.52)$$

and \mathcal{K}_c is defined in (3.10), \mathcal{D}_k^2 is defined in Lemma 2, \tilde{h}_k , \mathcal{D}_k^1 is defined in Lemma 3, and \hat{h}_{k+1} is defined in Lemma 4.

Proof. We can not directly apply the three lemma to estimate the three parts in (3.33). The reason is that $J_{\mathcal{U}}v \neq v_h$, which is the direct interpolation of v according to \mathcal{T}^h . The way to circumvent this difficulty is by defining

$$w := v - \sum_{k=1}^K \frac{1}{2} (x_{k+1} - x_{k-1}) v(x_k) \text{ and } w_h := I_h w = J_{\mathcal{U}}v, \quad (3.53)$$

and noting that

$$\langle f, J_{\mathcal{U}}v \rangle_h - \langle f, v \rangle_{\varepsilon} = \langle f, w_h \rangle_h - \langle f, w \rangle_{\varepsilon} - \langle f, C \rangle_{\varepsilon} = \langle f, w_h \rangle_h - \langle f, w \rangle_{\varepsilon}, \quad (3.54)$$

and $w'(x) = v'(x) \forall x \in \mathbb{R}$. Then by the three lemma, we have

$$|\langle f, J_{\mathcal{U}}v \rangle_h - \langle f, v \rangle_{\varepsilon}| = |\langle f, w_h \rangle_h - \langle f, w \rangle_{\varepsilon}| \leq \left\{ \sum_{k \in \mathcal{K}_c} \eta_k^{f^2} \right\}^{\frac{1}{2}} \|w'\|_{L^2[0,1]} = \left\{ \sum_{k \in \mathcal{K}_c} \eta_k^{f^2} \right\}^{\frac{1}{2}} \|v'\|_{L^2[0,1]}, \quad (3.55)$$

which establishes the estimate in the theorem. \square

4. STABILITY

Stability of the QC approximation is the second key ingredient for deriving an a posteriori error bounds. Since we would like to bound the error of the deformation gradient in L^2 -norm, we derive the L^2 stability estimate in this section. The procedure of deriving the a posteriori stability condition largely follows that of the a priori stability condition in [8].

For an a posteriori error analysis, the natural notion of stability for energy minimization problem is the coercivity(or, positivity) of the atomistic Hessian at the projected QC solution $J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}}$:

$$E''_{\text{a}}(J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}})[v, v] \geq c_{\text{a}}(y_{\text{qc}}) \|v\|_{L^2[0,1]}^2 \quad \forall v \in \mathcal{U}, \quad (4.1)$$

for some constant $c_{\text{a}}(y_{\text{qc}}) > 0$. To avoid notational difficulty, we vectorize the above inequality and work on $\mathcal{U}^{\varepsilon}$ instead. Let $J_{\mathcal{U}_{\text{qc}}}\mathbf{y}^{\text{qc}}$ be the vectorization of $J_{\mathcal{U}_{\text{qc}}}y_{\text{qc}}$, then (4.1) is equivalent to

$$E''_{\text{a}}(J_{\mathcal{U}_{\text{qc}}}\mathbf{y}^{\text{qc}})[\mathbf{v}, \mathbf{v}] \geq c_{\text{a}}(J_{\mathcal{U}_{\text{qc}}}\mathbf{y}^{\text{qc}}) \|\mathbf{v}\|_{\ell_{\varepsilon}^2}^2 \quad \forall \mathbf{v} \in \mathcal{U}. \quad (4.2)$$

In the remainder of this section, we derive the explicit condition on \mathbf{y}^{qc} such that (4.2) holds.

The Hessian operator of the atomistic model is given by

$$E''_{\text{a}}(\mathbf{y})[\mathbf{v}, \mathbf{v}] = \varepsilon \sum_{\ell=1}^N \phi''(y'_{\ell}) |v'_{\ell}|^2 + \varepsilon \sum_{\ell=1}^N \phi''(y'_{\ell} + y'_{\ell+1}) |v'_{\ell} + v'_{\ell+1}|^2 \quad \forall \mathbf{y} \in \mathcal{Y}.$$

We note that the 'non-local' Hessian terms $|v'_{\ell} + v'_{\ell+1}|^2$ can be rewritten in terms of the 'local' terms $|v'_{\ell}|^2$ and $|v'_{\ell+1}|^2$ and a strain-gradient correction,

$$|v'_{\ell} + v'_{\ell+1}|^2 = 2|v'_{\ell}|^2 + 2|v'_{\ell+1}|^2 - \varepsilon^2 |v''_{\ell}|^2.$$

Using this formula, we can rewrite the Hessian in the form

$$E''_{\mathbf{a}}(\mathbf{y})[\mathbf{v}, \mathbf{v}] = \varepsilon \sum_{\ell=1}^N A_{\ell} |v'_{\ell}|^2 + \varepsilon \sum_{\ell=1}^N B_{\ell} |v''_{\ell}|^2,$$

where

$$\begin{aligned} A_{\ell}(\mathbf{y}) &= \phi''(y'_{\ell}) + 2\phi''(y'_{\ell-1} + y'_{\ell}) + 2\phi''(y'_{\ell} + y'_{\ell+1}) \\ B_{\ell}(\mathbf{y}) &= -\phi''(y'_{\ell} + y'_{\ell+1}). \end{aligned} \quad (4.3)$$

Recall our assumption that ϕ is convex in $(0, r_*)$ and concave in $(r_*, +\infty)$. For typical pair interaction potentials, $y'_{\ell} < r_*/2$ can only be achieved under extreme compressive forces. Since, under such extreme conditions a pair potential may be an inappropriate model to employ anyhow, it is not too restrictive to assume that the projected QC solution $J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}$ satisfies

$$(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_{\ell} \geq r_*/2 \quad \forall \ell \in \mathbb{Z}.$$

As a result of this assumption, and the properties of ϕ , we have $-\phi''(y'_{\ell} + y'_{\ell+1}) \geq 0 \quad \forall \ell \in \mathbb{Z}$ and thus $B_{\ell} \geq 0 \quad \forall \ell \in \mathbb{Z}$.

As an immediate consequence we obtain the following lemma, which gives sufficient conditions under which the a posteriori stability of QC approximation can be guaranteed.

Lemma 6. *Let $J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}} \in \mathcal{Y}^{\varepsilon}$ satisfies $\min_{\ell} (J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_{\ell} \geq r_*/2$; then,*

$$E''_{\mathbf{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[\mathbf{v}, \mathbf{v}] \geq A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}^2 \quad \forall \mathbf{v} \in \mathcal{U}, \quad \text{where} \quad A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) = \min_{\ell=1, \dots, N} A_{\ell}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}).$$

The coefficients $A_{\ell}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})$ are defined in (4.3).

Proof. If $\min_{\ell} (J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_{\ell} \geq r_*/2$, then

$$E''_{\mathbf{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[\mathbf{v}, \mathbf{v}] \geq \varepsilon \sum_{\ell=1}^N A_{\ell}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) |v'_{\ell}|^2 \geq A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) \varepsilon \sum_{\ell=1}^N |v'_{\ell}|^2 = A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) \|\mathbf{v}'\|_{\ell_{\varepsilon}^2}^2. \quad \square$$

Before we present the main theorem and its proof in the next section, we state a useful auxiliary result: a local Lipschitz bound on $E''_{\mathbf{a}}$. The proof of this Lipschitz bound is straightforward and is therefore omitted.

Lemma 7. *Let $\mathbf{y}, \mathbf{z} \in \mathcal{Y}^{\varepsilon}$ such that $\min_{\ell} y'_{\ell} \geq \mu$ and $\min_{\ell} z'_{\ell} \geq \mu$ for some constant $\mu > 0$, then*

$$|\{\mathcal{E}''_{\mathbf{a}}(\mathbf{y}) - \mathcal{E}''_{\mathbf{a}}(\mathbf{z})\}[\mathbf{v}, \mathbf{w}]| \leq C_{\text{Lip}} \|\mathbf{y}' - \mathbf{z}'\|_{\ell_{\varepsilon}^{\infty}} \|\mathbf{v}'\|_{\ell_{\varepsilon}^2} \|\mathbf{w}'\|_{\ell_{\varepsilon}^2} \quad \forall \mathbf{v}, \mathbf{w} \in \mathcal{U},$$

where $C_{\text{Lip}} = M_3([\mu, +\infty)) + 8M_3([2\mu, +\infty))$ and $M_i(S) = \max_{\xi \in S} |\phi^i(\xi)|$.

5. A POSTERIORI ERROR ESTIMATES

5.1. The a posterior error estimates for the deformation gradient. The error we estimate is $e := y_{\mathbf{a}} - J_{\mathcal{U}_{\text{qc}}} y_{\text{qc}}$ in the $\mathcal{U}^{1,2}$ -norm, as for $y_1, y_2 \in \mathcal{Y}$, $y_1 - y_2 \in \mathcal{U}$. To avoid technicalities associated with the nonlinearity of our models, we make an a priori assumption: we assume the existence of the atomistic and QC solutions and make a mild requirement on their smoothness and closeness (cf. (5.1)).

Theorem 8. *Let y_{qc} be a solution of the QC problem (2.25) whose gradients are such that $\min_{\ell} (J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_{\ell} \geq r_*/2 \quad \forall \ell \in \mathbb{Z}$ and $A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) > 0$, where A_* is defined in the statement of*

Lemma 6. Suppose, further, that y^a is a solution of the atomistic model (2.8) such that, for some $\tau > 0$,

$$\|(y^a - J_{\mathcal{U}_{\text{qc}}} y_{\text{qc}})'\|_{L^\infty[0,1]} = \|(\mathbf{y}^a - J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'\|_{\ell_\varepsilon^\infty} \leq \tau. \quad (5.1)$$

Then, if τ is sufficiently small, we have the error estimate

$$\|y^a - J_{\mathcal{U}_{\text{qc}}} y_{\text{qc}}\|_{L^2[0,1]} = \|(\mathbf{y}^a - J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'\|_{\ell_\varepsilon^2} \leq \frac{2}{A_*(\mathbf{y}^a)} (\mathcal{E}_{\text{store}}(y_{\text{qc}}) + \mathcal{E}_{\text{ext}}(f)), \quad (5.2)$$

where the functional of the residual of the stored energy $\mathcal{E}_{\text{store}}(\cdot)$ is defined in (3.11) and the functional of the approximation error for the external forces $\mathcal{E}_{\text{ext}}(\cdot)$ is defined in (3.51).

Proof. From the mean value theorem we deduce that there exists $\boldsymbol{\theta} \in \text{conv}\{\mathbf{y}^a, J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}\}$ such that

$$\begin{aligned} E''_{\text{a}}(\boldsymbol{\theta})[\mathbf{e}, \mathbf{e}] &= E'_{\text{a}}(\mathbf{y}^a)[\mathbf{v}] - E'_{\text{qc}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[J_{\mathcal{U}} \mathbf{v}] \\ &= (\mathcal{E}'_{\text{a}}(\mathbf{y}^a)[\mathbf{v}] - \mathcal{E}'_{\text{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[J_{\mathcal{U}} \mathbf{v}]) \\ &\quad - (\langle \mathbf{f}, \mathbf{v} \rangle_\varepsilon - \langle \mathbf{f}, J_{\mathcal{U}} \mathbf{v} \rangle_h). \end{aligned}$$

The first group was analyzed in section 3.2 Theorem 1 and the second group was analyzed in section 3.3 Theorem 5. Inserting these estimates we arrive at

$$E''_{\text{a}}(\boldsymbol{\theta})[\mathbf{e}, \mathbf{e}] \leq (\mathcal{E}_{\text{store}}(y^{\text{qc}}) + \mathcal{E}_{\text{ext}}(f)) \|\mathbf{e}'\|_{\ell_\varepsilon^2}. \quad (5.3)$$

It remains to prove a lower bound on $\mathcal{E}''_{\text{a}}(\boldsymbol{\theta})[\mathbf{e}, \mathbf{e}]$. From our assumption that $\min(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_\ell \geq r_*/2$, and from (5.1) it follows that

$$\min_\ell \theta'_\ell \geq r_*/2 - \tau.$$

Assuming that τ is sufficiently small, e.g., $\tau \leq \tau_1 := \frac{1}{4} \min_\ell (J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_\ell$, we can apply Lemma 7 to deduce that

$$\begin{aligned} \mathcal{E}''_{\text{a}}(\boldsymbol{\theta})[\mathbf{e}, \mathbf{e}] &\geq \mathcal{E}''_{\text{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[\mathbf{e}, \mathbf{e}] - C_{\text{Lip}} \|(\boldsymbol{\theta} - \mathbf{y}^a)\|_{\ell_\varepsilon^\infty} \|\mathbf{e}'\|_{\ell_\varepsilon^2}^2 \\ &\geq \mathcal{E}''_{\text{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[\mathbf{e}, \mathbf{e}] - C_{\text{Lip}} \tau \|\mathbf{e}'\|_{\ell_\varepsilon^2}^2, \end{aligned} \quad (5.4)$$

where C_{Lip} may depend on τ_1 .

We can now apply our stability analysis in Section 4. Since $(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})'_\ell \geq r_*/2$ for all ℓ , Lemma 6 implies that

$$\mathcal{E}''_{\text{a}}(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})[\mathbf{e}, \mathbf{e}] \geq A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) \|\mathbf{e}'\|_{\ell_\varepsilon^2}^2,$$

which, combined with (5.3) and (5.4), yields

$$(A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}}) - C_{\text{Lip}} \tau) \|\mathbf{e}'\|_{\ell_\varepsilon^2}^2 \leq \mathcal{E}''_{\text{a}}(\boldsymbol{\theta})[\mathbf{e}, \mathbf{e}] \leq (\mathcal{E}_{\text{store}}(y_{\text{qc}}) + \mathcal{E}_{\text{ext}}(f)) \|\mathbf{e}'\|_{\ell_\varepsilon^2}.$$

Dividing through by $\|\mathbf{e}'\|_{\ell_\varepsilon^2}$, and assuming that $\tau \leq \min(\tau_1, \tau_2)$ where $\tau_2 = A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})/(2C_{\text{Lip}})$, we deduce that

$$\frac{A_*(J_{\mathcal{U}_{\text{qc}}} \mathbf{y}^{\text{qc}})}{2} \|\mathbf{e}'\|_{\ell_\varepsilon^2} \leq (\mathcal{E}_{\text{store}}(y_{\text{qc}}) + \mathcal{E}_{\text{ext}}(f)),$$

which concludes the proof of the a posteriori error estimate for the deformation gradient. \square

5.2. The a posteriori error estimate for the energy. Besides the deformation gradient, the energy of the system is another quantity of interest. In this section, we derive an a posteriori error estimator for the energy difference between the atomistic model and the QC approximation, namely,

$$E_a(y^a) - E_{qc}(y_{qc}). \quad (5.5)$$

To analyze this difference, we decompose (5.5) as

$$|E_a(y^a) - E_{qc}(y_{qc})| = |E_a(y^a) - E_a(J_{\mathcal{U}_{qc}}y_{qc})| + |E_a(J_{\mathcal{U}_{qc}}y_{qc}) - E_{qc}(y_{qc})|. \quad (5.6)$$

We then analyze the two groups separately.

To analyze the first group, we have the following Lemma.

Lemma 9. *Let $y, z \in \mathcal{Y}$ and $\mathbf{y}, \mathbf{z} \in \mathcal{Y}^\varepsilon$ be their vectorizations, such that $\min_\ell y'_\ell \geq \mu$ and $\min_\ell z'_\ell \geq \mu$ for some constant $\mu > 0$, and $y \in \operatorname{argmin} E_a(\mathcal{Y})$. Let $\mathbf{e} = \mathbf{y} - \mathbf{z}$, then*

$$|E_a(\mathbf{y}) - E_a(\mathbf{z})| \leq C_{\text{Lip}}^E \|\mathbf{e}'\|_{\ell_\varepsilon^2}^2, \quad (5.7)$$

where $C_{\text{Lip}}^E = \frac{1}{2}M_2([\mu, +\infty)) + 2M_3([2\mu, +\infty))$, where $M_i(S) = \max_{\xi \in S} |\phi^i(\mathcal{S})|$.

Proof. We first rewrite the difference of the total energy as the summation of the differences of the stored energy and that of the external energy:

$$E_a(\mathbf{y}) - E_a(\mathbf{z}) = (\mathcal{E}_a(\mathbf{y}) - \mathcal{E}_a(\mathbf{z})) - (\langle \mathbf{f}, \mathbf{z} \rangle_\varepsilon - \langle \mathbf{f}, \mathbf{y} \rangle_\varepsilon)$$

For the difference of the stored energy, we have

$$\begin{aligned} \mathcal{E}_a(\mathbf{y}) - \mathcal{E}_a(\mathbf{z}) &= \varepsilon \sum_{\ell=1}^N [\phi(y'_\ell) - \phi(z'_\ell)] + \varepsilon \sum_{\ell=1}^N [\phi(y'_\ell + y'_{\ell+1}) - \phi(z'_\ell + z'_{\ell+1})] \\ &= \varepsilon \sum_{\ell=1}^N [\phi'(y'_\ell)e'_\ell - \frac{1}{2}\phi''(\xi_\ell^1)e_\ell'^2] \\ &\quad + \varepsilon \sum_{\ell=1}^N [\phi'(y'_\ell + y'_{\ell+1})(e'_\ell + e'_{\ell+1}) - \frac{1}{2}\phi''(\xi_\ell^2)(e'_\ell + e'_{\ell+1})^2] \\ &= \mathcal{E}'_a(\mathbf{y})[\mathbf{e}] - \frac{1}{2}\varepsilon \sum_{\ell=1}^N \phi''(\xi_\ell^1)e_\ell'^2 - \frac{1}{2}\varepsilon \sum_{\ell=1}^N \phi''(\xi_\ell^2)(e'_\ell + e'_{\ell+1})^2, \end{aligned}$$

where $\xi_\ell^1 \in \operatorname{conv}\{y'_\ell, z'_\ell\}$ and $\xi_\ell^2 \in \operatorname{conv}\{y'_\ell + y'_{\ell+1}, z'_\ell + z'_{\ell+1}\}$.

For the difference of the energy caused by the external forces, we have

$$\langle \mathbf{f}, \mathbf{z} \rangle_\varepsilon - \langle \mathbf{f}, \mathbf{y} \rangle_\varepsilon = -\langle \mathbf{f}, \mathbf{e} \rangle_\varepsilon = -\mathcal{E}'_a(\mathbf{y})[\mathbf{e}],$$

by the first optimality condition of $y \in \operatorname{argmin} E_a(\mathcal{Y})$. It is then easy to obtain the estimate stated in the Lemma by using Cauchy-Schwarz inequality to the non-local term. \square

Lemma 10. *For $y_h \in \mathcal{Y}_{qc}$ and $y'_h(x) > 0$, we have*

$$|E_a(J_{\mathcal{U}_{qc}}y_h) - E_{qc}(y_h)| \leq \sum_{k \in \mathcal{K}_c} \eta_{E_k}^e + \eta_{E_k}^f, \quad (5.8)$$

where

$$\eta_k^e = \frac{1}{2} \sum_{j=-1}^1 [[\phi]]_{\ell_{k-1}+j} + \frac{1}{2} \sum_{j=-1}^1 [[\phi]]_{\ell_k+j}, \quad (5.9)$$

if $k \in \mathcal{K}'_c$,

$$\eta_k^e = \sum_{j=-1}^1 [[\phi]]_{\ell_{La_i}+j} + \frac{1}{2} \sum_{j=-1}^1 [[\phi]]_{\ell_{k-1}+j}, \quad (5.10)$$

if $k = La_i$ for some $i \in \{1, 2, \dots, M\}$, and

$$\eta_k^e = \sum_{j=-1}^1 [[\phi]]_{\ell_{Ra_i}+j} + \frac{1}{2} \sum_{j=-1}^1 [[\phi]]_{\ell_k+j}, \quad (5.11)$$

if $k = Ra_i$ for some $i \in \{1, 2, \dots, M\}$. $[[\phi]]_{\ell_k}$'s and $\eta_{E_k}^f$'s will be defined in the proof.

Proof. We first decompose the energy difference to two parts:

$$E_a(J_{\mathcal{U}_{qc}} y_h) - E_{qc}(y_h) = (\mathcal{E}_a(J_{\mathcal{U}_{qc}} y_h) - \mathcal{E}_{qc}(y_h)) - (\langle f, J_{\mathcal{U}_{qc}} y_h \rangle_\varepsilon - \langle f_h, y_h \rangle_h).$$

We first analyze the energy difference of the stored energy. Since $r_b D_b J_{\mathcal{U}_{qc}} y_h = r_b D_b y_h$, we have

$$\mathcal{E}_a(J_{\mathcal{U}_{qc}} y_h) = \sum_{b \in \mathcal{B}} a_b(J_{\mathcal{U}_{qc}} y_h) = \sum_{b \in \mathcal{B}} \varepsilon \phi(r_b D_b J_{\mathcal{U}_{qc}} y_h) = \sum_{b \in \mathcal{B}} \varepsilon \phi(r_b D_b y_h), \quad (5.12)$$

and

$$\mathcal{E}_{qc}(y_h) = \sum_{b \in \mathcal{B}} [a_b(y_h) + c_b(y_h)] = \sum_{b \in \mathcal{B}} \left[\frac{|b \cap \Omega_a|}{r_b} \phi(r_b D_{b \cap \Omega_a} y) + \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \right]. \quad (5.13)$$

We analyze the energy difference bond by bond,

If $b \subset \Omega_a$, then

$$a_b(y_h) + c_b(y_h) = a_b(y_h) = \varepsilon \phi(r_b D_b y_h) = a_b(J_{\mathcal{U}_{qc}} y_h),$$

and the energy difference in this bond is thus 0.

If $b \subset \Omega_c \cap T_k$ for some $k \in \mathcal{K}_c$, then $|b \cap \Omega_a| = 0$ and

$$\begin{aligned} a_b(J_{\mathcal{U}_{qc}} y_h) - [a_b(y_h) + c_b(y_h)] &= a_b(J_{\mathcal{U}_{qc}} y_h) - c_b(y_h) \\ &= \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y_h(x)) \, dx \\ &= \frac{1}{r_b} \int_b [\phi(r_b D_b y_h) - \phi(\nabla_{r_b} y_h(x))] \, dx. \end{aligned} \quad (5.14)$$

Since y_h is affine on T_k , $\nabla_{r_b} y(x) = r_b D_b y_h$ and subsequently, (5.14) is 0.

We are left with the interaction bonds crossing the atomistic-continuum interface and the boundaries of the elements in the continuum region. Again because of its tediousness, we leave the detail of this analysis to the Appendix and only give the results here:

$$\mathcal{E}_a(J_{\mathcal{U}_{qc}} y_h) - \mathcal{E}_{qc}(y_h) = \sum_{i=1}^M \sum_{j=-1}^1 [[\phi]]_{\ell_{La_i}+j} + \sum_{i=1}^M \sum_{j=-1}^1 [[\phi]]_{\ell_{Ra_i}+j} + \sum_{k \in \mathcal{K}'_c} \sum_{j=-1}^1 [[\phi]]_{\ell_k+j}. \quad (5.15)$$

For $k = La_i$ where $i \in \{1, 2, \dots, M\}$, we have

$$[[\phi]]_{\ell_k} = \varepsilon \{ \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) - \theta_k \phi(y'_h|_{T_k}) \}, \quad (5.16)$$

$$[[\phi]]_{\ell_{k-1}} = 2\varepsilon \{ \phi((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi(2y'_h|_{T_{k+1}}) - (1 + \theta_k) \phi(2y'_h|_{T_k}) \}. \quad (5.17)$$

and

$$[[\phi]]_{\ell_{k+1}} = 2\varepsilon \left\{ \phi(y'_h|_{T_{k+2}} + \theta_k y'_h|_{T_k} + (1 - \theta_k) y'_h|_{T_{k+1}}) \right. \\ \left. - (2 - \theta_k) \phi\left(\frac{2}{2 - \theta_k} y'_h|_{T_{k+2}} + \frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}}\right) - \theta_k \phi(2y'_h|_{T_k}) \right\}. \quad (5.18)$$

For $k = R_{a_i}$ where $i \in \{1, 2, \dots, M\}$, we have

$$[[\phi]]_{\ell_k} = \varepsilon \left\{ \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) \right\}, \quad (5.19)$$

$$[[\phi]]_{\ell_{k-1}} = 2\varepsilon \left\{ \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) \right. \\ \left. - (1 - \theta_k) \phi(2y'_h|_{T_{k+1}}) - (1 + \theta_k) \phi\left(\frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}\right) \right\}, \quad (5.20)$$

and

$$[[\phi]]_{\ell_{k+1}} = 2\varepsilon \left\{ \phi((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (2 - \theta_k) \phi(2y'_h|_{T_{k+1}}) - \theta_k \phi(2y'_h|_{T_k}) \right\}. \quad (5.21)$$

For $k \in \mathcal{K}'_c$, we have

$$[[\phi]]_{\ell_k} = \varepsilon \left\{ \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) - \theta_k \phi(y'_h|_{T_k}) \right\}, \quad (5.22)$$

$$[[\phi]]_{\ell_{k-1}} = \frac{1}{2}\varepsilon \left\{ 2\phi((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - (1 - \theta_k) \phi(2y'_h|_{T_{k+1}}) - (1 + \theta_k) \phi(2y'_h|_{T_k}) \right\}, \quad (5.23)$$

and

$$[[\phi]]_{\ell_{k+1}} = \frac{1}{2}\varepsilon \left\{ 2\phi((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(2y'_h|_{T_{k+1}}) - (2 - \theta_k) \phi(2y'_h|_{T_k}) \right\}. \quad (5.24)$$

We then analyze the energy difference caused by the external forces. The energy difference is given by

$$\langle f, J_{\mathcal{U}_{qc}} u_h \rangle_\varepsilon - \langle f, u_h \rangle_h = \langle f, u_h \rangle_\varepsilon - \langle f, u_h \rangle_h,$$

since $J_{\mathcal{U}_{qc}} u_h = u_h + C$ for some constant C and $\langle f, C \rangle_\varepsilon = 0 \ \forall C$. We decompose this energy difference to each element and write it as

$$|\langle f, u_h \rangle_\varepsilon - \langle f, u_h \rangle_h| \leq \sum_{k=1}^K \eta_{Ek}^f, \quad (5.25)$$

where

$$\eta_{Ek}^f = \left| (1 - \theta_k) \frac{1}{2} \varepsilon (f_{\ell_{k-1}} u_{\ell_{k-1}} + f_{\ell_{k-1}+1} u_{\ell_{k-1}+1}) + \frac{1}{2} \sum_{\ell=\ell_{k-1}+2}^{\ell_k-1} \varepsilon (f_\ell u_\ell + f_{\ell+1} u_{\ell+1}) \right. \\ \left. + \theta \frac{1}{2} \varepsilon (f_{\ell_k} u_{\ell_k} + f_{\ell_k+1} u_{\ell_k+1}) \right\} - \sum_{k=1}^K \frac{1}{2} (x_k - x_{k-1}) [f(x_{k-1}) y(x_{k-1}) + f(x_k) y(x_k)] \Big|, \quad (5.26)$$

where $f_\ell = f(\ell\varepsilon)$ and $u_\ell = u(\ell\varepsilon)$. □

6. NUMERICAL EXPERIMENTS

In this section, we present numerical experiments to illustrate our analysis. Throughout this section we fix $F = 1$, $N = 8193$, and let ϕ be the Morse potential

$$\phi(r) = \exp(-2\alpha(r-1)) - 2\exp(-\alpha(r-1)),$$

with the parameter $\alpha = 5$.

For our benchmark problem, we defined the external force \mathbf{f} to be

$$f_\ell = \begin{cases} -0.1 \left\{ 1 - \frac{|\ell - \frac{N-1}{2}|}{\frac{N-1}{2}} \right\} \frac{N}{|\ell - \frac{N-1}{2} - 0.5|}, & \text{for } \ell \leq \frac{N-1}{2}, \\ 0.1 \left\{ 1 - \frac{\ell - \frac{N-1}{2}}{\frac{N-1}{2}} \right\} \frac{N}{|\ell - \frac{N-1}{2} - 0.5|}, & \text{for } \ell \geq \frac{N-1}{2} + 1. \end{cases}$$

We briefly explain the meaning of the external force. On each atom, the external force is a product of three components. The third component, namely $\frac{N}{|\ell - \frac{N-1}{2} - 0.5|}$ is essentially $\frac{1}{r_\ell}$ where r_ℓ is the distance between an atom and the center of this atomistic chain located at $\frac{N-1}{2} + 0.5$. This non-linear force will create a defect in the middle of the chain but affect little in the far field. The second component, namely $1 - \frac{|\ell - \frac{N-1}{2}|}{\frac{N-1}{2}}$, adds a decay of the first component and in particular, it is 0 when $\ell = N$, which prevents the 'kink' of the force on the boundary due to a rapid change of the sign of the force that will leads to non-smooth deformation gradient that should be contained in the atomistic region. The first component, which is the constant 0.1, is to rescale the force so that the solution of this problem is stable.

We solve for the atomistic problem and consider the solution to be the accurate solution. We then solve for the QC problem on different meshes generated by the mesh refinement schemes.

We show two relative errors against the number of degrees of freedom. The first one is the error of the deformation gradient in L_2 -norm over the L_2 -norm of the difference between the deformation gradient of the atomistic solution and the homogeneous state, which is defined by

$$e_{\text{deformation}} := \frac{\|y'_{\text{qc}} - y'_a\|_{L^2[0,1]}}{\|y'_a - Fx\|_{L^2[0,1]}}. \quad (6.1)$$

The second relative error is the absolute value of the energy difference of the atomistic solution and the QC solution over the absolute value of the energy change of the atomistic solution from the homogeneous state, which is defined by

$$e_{\text{energy}} := \frac{|E_a(y_a) - E_{\text{qc}}(y_{\text{qc}})|}{|E_a(y_a) - E_a(Fx)|}. \quad (6.2)$$

Before we present the plots of the errors, we first introduce the mesh generating schemes.

6.1. Mesh Construction. To avoid unnecessary technical difficulty in the mesh refinement algorithm, we assume that the defect core is already captured in the middle of the chain. There are three mesh generating schemes we use.

The first mesh generating scheme is derived in Section 7.1 of [6] using calculus of variations. From this analysis, we get that the (quasi-)optimal mesh size in the continuum region, with the restriction that the atomistic region is symmetric and has K atoms on each side, is given by

$$h(r) = \left(\frac{f(K\varepsilon)}{f(r)} \frac{r}{K\varepsilon} \right)^{\frac{2}{3}}. \quad (6.3)$$

Since the mesh size can not change continuously and we restrict the smallest mesh size in the continuum region to be 2ε , we use the following algorithm to generate this mesh (we only list the case on the right hand side of the atomistic region):

Algorithm 1.

- (1) Set atom $\frac{N-1}{2} + 1$ to be the middle of the atomistic region.
- (2) Choose K so that there are K atoms on each side of the atomistic region.
- (3) Choose h to be 2ε for every element on the right hand side of the atomistic region until $h(r) > 2\varepsilon$, where r is the distance between the right boundary of the previous element and the middle of the atomistic region.
- (4) Choose h according to (6.3) until the right boundary of the newly created element is out of the right limit of the chain.

□

The second mesh generating scheme is essentially a mesh refinement process according to the error estimator with respect to the deformation gradient according to Lemma 2, Lemma 3 and Lemma 4. The mesh refinement algorithm is stated as follows:

Algorithm 2.

- (1) Set atom $\frac{N-1}{2} + 1$ to be the middle of the atomistic region.
- (2) Choose 5 atoms on each side of the atomistic region.
- (3) Divide the left and the right part of the continuum region into two equally large element
- (4) Compute the QC solution on this mesh and then compute the squared error indicator of each element η_i and sort these indicators according to its value.
- (5) Bisect the first M sorted elements such that

$$\sum_{i=1}^{M-1} \eta_i^2 \leq 0.5\eta^2 \text{ and } \sum_{i=1}^M \eta_i^2 \geq 0.5\eta^2, \quad (6.4)$$

where η_i is the error estimator of each element defined by

$$\eta_i^{deformation} = [(\eta_i^e)^2 + (\eta_i^f)^2]^{\frac{1}{2}} / \frac{A_*(J\mathcal{U}_{qc}\mathbf{y}^{qc})}{2}. \quad (6.5)$$

If the element is near the atomistic region, merge the element into the atomistic region.

- (6) If the resulting mesh reaches the maximal number of degrees of freedom, stop the process, else, go to Step 4.

□

The third mesh generating scheme is the mesh refinement process according to the error estimator with respect to the energy which is defined by

$$\eta_i^{energy} = C_{Lip}^E (\eta_i^{deformation})^2 + \eta_{E_k}^e + \eta_{E_k}^f, \quad (6.6)$$

for each element and the refinement algorithm is exactly the same.

In short, the first and second mesh generating schemes tend to minimize the error in the deformation gradient and the third one tends to minimize the error in the total energy.

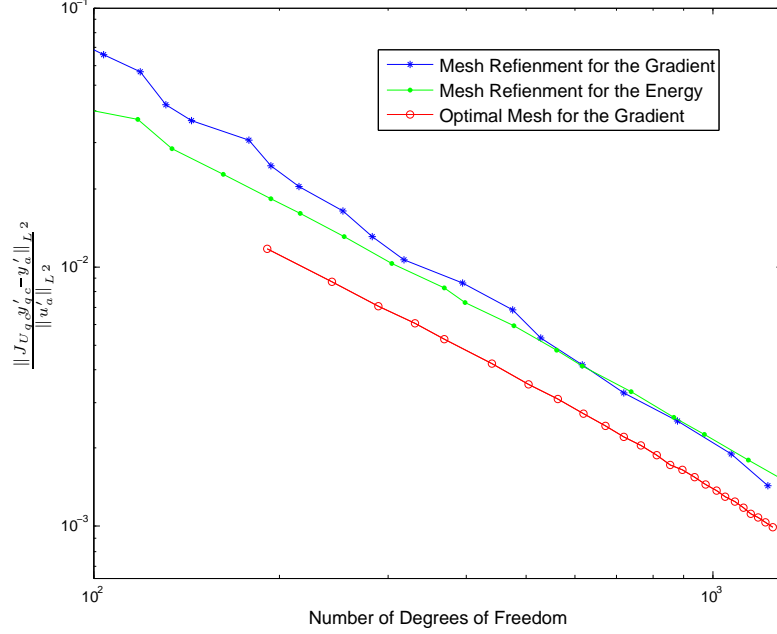


FIGURE 1. Relative Error of the Gradient

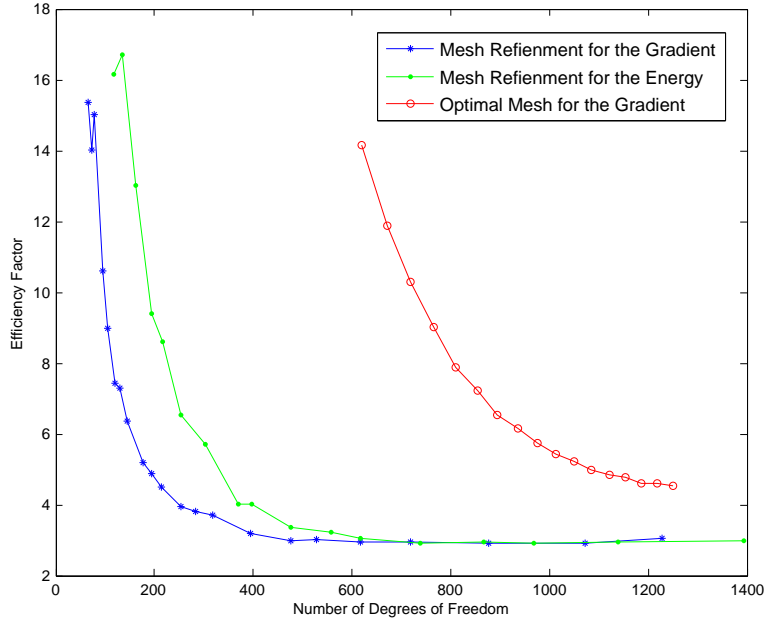


FIGURE 2. Efficiency Factor of the Gradient

6.2. Numerical Results. We compare the relative errors defined in 6.1 and 6.2. We plot the relative errors against the number of degrees of freedom with respect to the meshes generated.

Figure 1 shows that the pre-defined optimal mesh performs better than the two mesh refinement strategies for a fix number of degrees of freedom. The possible reason for this is that, due to some technical difficulty in coding, both of the mesh refinement algorithms tend to produce larger atomistic region by merging the elements in the continuum region to the atomistic region and create some unnecessary degrees of freedom. For the two mesh refinement strategies, the one according to the gradient error indicator perform better asymptotically.

Figure 2 shows the efficiency factor of the error estimator of the deformation gradient. It shows that the efficiency factor is comparatively large but decreases as the number of degrees of freedom increases and finally become stable. The reason for this phenomenon lies in the form of the external force. One can show that if the external force takes the form of $f(r) = \frac{1}{r}$, where r is the distance to the centre of the defect, then the residual due to the external force is of order h^2 as opposed to order h in general which is achieved by our analysis. As a result, our estimate exaggerate the real error by $\frac{1}{h}$ for this particular external force. This phenomenon gradually disappear as the continuum region moves apart from the centre of the defect since the influence of this exaggeration is eliminated as the external force tends to 0 when it is away from the centre of the defect, which makes the residual of the solved energy become the leading error term. It can also well explain the fact that the efficiency of the estimate is better for the mesh refinement strategies than the pre-defined mesh for a certain number of degrees of freedom, as the two mesh refinement algorithms tend to put more atoms in the atomistic region, i.e., the continuum region is further away from the centre of defect than that of the pre-defined mesh.

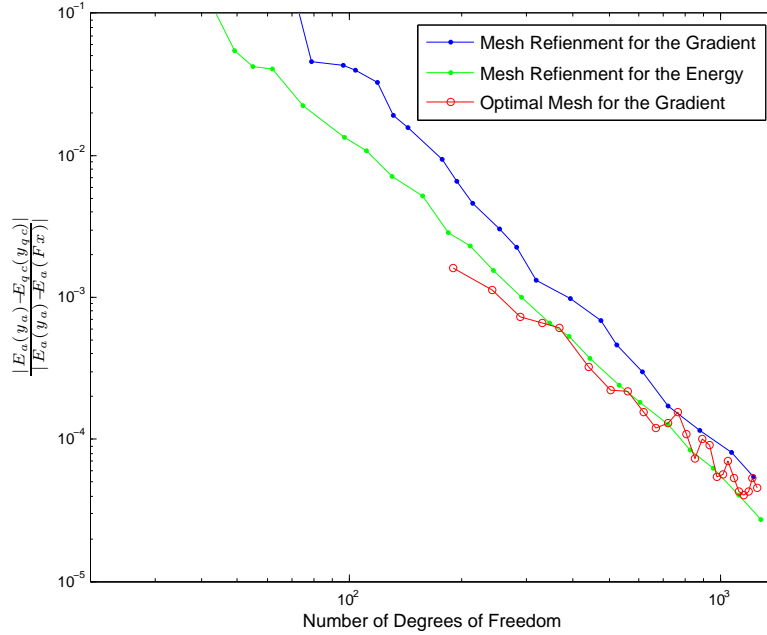


FIGURE 3. Relative Error of the Total Energy

Figure 3 shows that the refinement based on the energy error performs the best among all the three mesh generating schemes.

Figure 4 shows the efficiency factor of the error estimator of the energy. For the same reason, this factor decreases as the number of degrees of freedom increases and finally becomes stable.

7. CONCLUSION

We have presented the a posteriori error estimates for the Consistent Energy-Based QC method in one dimension. The procedure of the estimate is the same as that in [8]. However, since the formulation of the QC problem is newly developed and is totally different from previous ones, new techniques have been developed and applied to deal with the difficulty in the analysis. Several results derived may be of independent interest and usefulness. In addition, the error

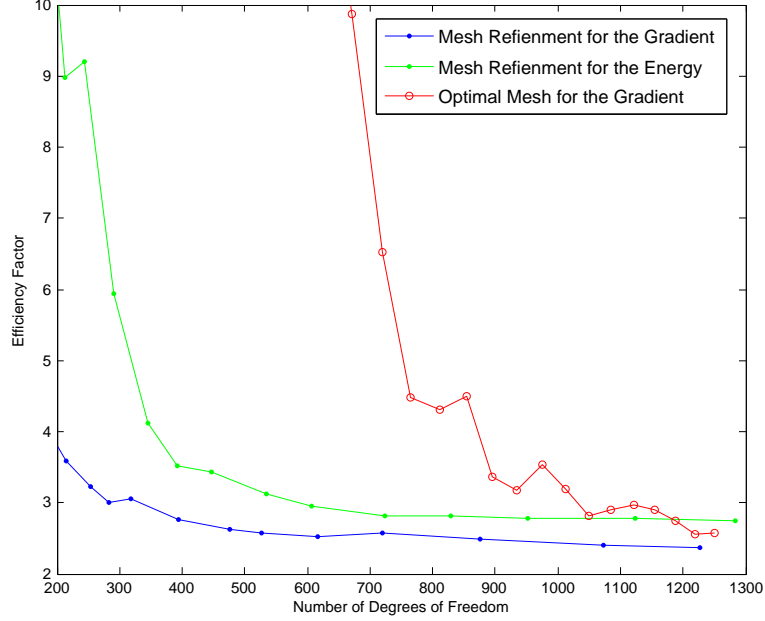


FIGURE 4. Efficiency Factor of the Energy

estimate of the total energy is also derived. Numerical experiments are also implemented to illustrate our analysis.

Particular interesting future work are the extension and the implementation of the a posteriori error estimate in higher dimensional problems. The difficulty lies in the complication of the formulation and the varied location of the interaction bonds. However, since a priori analysis for the two dimensional problem has been proposed [6], ways of circumventing these difficulties could be a source of reference.

APPENDIX A. DETAILED ANALYSIS FOR THE RESIDUALS OF THE STORED ENERGY

In this section, we provide the omitted detailed analysis for the residuals of the stored energy, namely

$$\mathcal{E}'_a(J_{\mathcal{U}_{qc}}y_h)[v] - \mathcal{E}'_{qc}(y_h)[J_{\mathcal{U}}[v]] \text{ and } \mathcal{E}_a(J_{\mathcal{U}_{qc}}y_h) - \mathcal{E}_{qc}(y_h),$$

where $y_h \in \mathcal{Y}_{qc}$, $y'_h(x) > 0 \forall x \in \mathbb{R}$ and $v \in \mathcal{U}$.

The idea is to find the differences defined by

$$\varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx, \quad (\text{A.1})$$

and

$$\varepsilon \phi(r_b D_b y_h) - |b \cap \Omega_a| r_b \phi(r_b D_{b \cap \Omega_a} y) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx, \quad (\text{A.2})$$

for each interaction bond b .

We have analyzed the cases that $b \in \Omega_a$ and $b \in T_k \cap \Omega_c$ and are left with the analysis for the cases that b is across the atomistic-continuum interface and the boundaries of the elements in the continuum region. There are three cases and in each case there are three subcases to be considered.

Case 1: b is across two adjacent elements $T_k, T_{k+1} \in \Omega_c$. In this case $|b \cap \Omega_a| = 0$ and the atomistic contribution of the interaction bond in the QC energy is 0.

Subcase 1: If $b = (\ell_k \varepsilon, (\ell_k + 1)\varepsilon)$, then $r_b = 1$, $b \cap T_k = [\ell_k \varepsilon, x_k^h]$, $b \cap T_{k+1} = [x_k^h, (\ell_k + 1)\varepsilon]$, $r_b D_b v = v'_{\ell_k+1}$ and

$$r_b D_b y_h = \frac{y_h((\ell_k + 1)\varepsilon) - y_h(\ell_k \varepsilon)}{\varepsilon} = (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}.$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\ &= \varepsilon \phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) v'_{\ell_k+1} - \frac{1}{r_b} \phi'(r_b y_h|_{T_{k+1}}) \int_{b \cap T_k} r_b v' \, dx - \frac{1}{r_b} \phi'(r_b y_h|_{T_k}) \int_{b \cap T_{k+1}} r_b v' \, dx \\ &= \varepsilon \left\{ \phi'(r_b D_b y_h) - (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) - \theta_k \phi'(\theta_k y'_h|_{T_k}) \right\} v'_{\ell_k+1}, \end{aligned}$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\ &= \varepsilon \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \int_{b \cap T_k} \phi(y'_h|_{T_k}) \, dx - \int_{b \cap T_{k+1}} \phi(y'_h|_{T_{k+1}}) \, dx \\ &= \varepsilon \left(\phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) \right). \end{aligned} \quad (\text{A.3})$$

Subcase 2: If $b = ((\ell - 1)\varepsilon, (\ell_k + 1)\varepsilon)$, then $r_b = 2$, $b \cap T_k = [(\ell_k - 1)\varepsilon, x_k^h]$, $b \cap T_{k+1} = [x_k^h, (\ell_k + 1)\varepsilon]$, $r_b D_b v = v'_{\ell_k+1} + v'_{\ell_k}$ and

$$r_b D_b y_h = \frac{y_h(\ell_k \varepsilon) - y_h((\ell_k - 1)\varepsilon)}{\varepsilon} = (1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}.$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\ &= \varepsilon \phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) (v'_{\ell_k+1} + v'_{\ell_k}) \\ & \quad - \frac{1}{r_b} \phi'(r_b y_h|_{T_{k+1}}) \int_{b \cap T_k} r_b v' \, dx - \frac{1}{r_b} \phi'(r_b y_h|_{T_k}) \int_{b \cap T_{k+1}} r_b v' \, dx \\ &= \varepsilon \left\{ [\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - \phi'(2y'_h|_{T_k})] v'_{\ell_k} \right. \\ & \quad \left. + [\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - (1 - \theta_k) \phi'(2y'_h|_{T_{k+1}}) - \theta_k \phi'(2y'_h|_{T_k})] v'_{\ell_k+1} \right\}, \end{aligned}$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\ &= \frac{1}{2} \varepsilon \left(2\phi((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - (1 + \theta_k) \phi(2y'_h|_{T_k}) - (1 - \theta_k) \phi(2y'_h|_{T_{k+1}}) \right). \end{aligned} \quad (\text{A.4})$$

Subcase 3: If $b = (\ell_k \varepsilon, (\ell_k + 2)\varepsilon)$, then $r_b = 2$, $b \cap T_k = [\ell_k \varepsilon, x_k^h]$, $b \cap T_{k+1} = [x_k^h, (\ell_k + 2)\varepsilon]$, $r_b D_b v = v'_{\ell_k+2} + v'_{\ell_k+1}$ and

$$r_b D_b y_h = \frac{y_h((\ell_k + 2)\varepsilon) - y_h(\ell_k \varepsilon)}{\varepsilon} = (2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}.$$

We have

$$\begin{aligned}
& \varepsilon \phi'(r_b D_b y_h) r_b D_b v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\
&= \varepsilon \phi'((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) (v'_{\ell_k+2} + v'_{\ell_k+1}) \\
&\quad - \frac{1}{r_b} \phi'(r_b y_h|_{T_{k+1}}) \int_{b \cap T_k} r_b v' \, dx - \frac{1}{r_b} \phi'(r_b y_h|_{T_k}) \int_{b \cap T_{k+1}} r_b v' \, dx \\
&= \varepsilon \left\{ [\phi'((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi'(2 y'_h|_{T_{k+1}}) - \theta_k \phi'(2 y'_h|_{T_k})] v'_{\ell_k+1} \right. \\
&\quad \left. + [\phi'((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \phi'(2 y'_h|_{T_{k+1}})] v'_{\ell_k+2} \right\},
\end{aligned}$$

and

$$\begin{aligned}
& \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\
&= \frac{1}{2} \varepsilon \left(2 \phi((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(2 y'_h|_{T_{k+1}}) - (2 - \theta_k) \phi(2 y'_h|_{T_k}) \right). \quad (\text{A.5})
\end{aligned}$$

Case 2: b is across the *left* atomistic-continuum interface of an atomistic region.

Subcase 1: If $b = (\ell_k \varepsilon, \ell_{k+1} \varepsilon)$, then $r_b = 1$, $b \cap \Omega_c = (\ell_k \varepsilon, x_k^h)$, $b \cap \Omega_a = (x_k^h, (\ell_k + 1) \varepsilon)$, $r_b D_b v = v'_{\ell_k+1}$ and

$$r_b D_b y_h = (1 - \theta_k) y_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}.$$

We have

$$\begin{aligned}
& \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\
&= \varepsilon \left[\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) - \theta_k \phi'(y'_h|_{T_k}) \right] v'_{\ell_k+1}, \quad (\text{A.6})
\end{aligned}$$

and

$$\begin{aligned}
& \varepsilon \phi(r_b D_b y_h) - |b \cap \Omega_a| r_b \phi(r_b D_{b \cap \Omega_a} y) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\
&= \varepsilon (\phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}})) \quad (\text{A.7})
\end{aligned}$$

Subcase 2: If $b = ((\ell_k - 1) \varepsilon, (\ell_k + 1) \varepsilon)$, then $r_b = 2$, $b \cap \Omega_c = ((\ell_k - 1) \varepsilon, x_k^h)$, $b \cap \Omega_a = (x_k^h, (\ell_k + 1) \varepsilon)$, $r_b D_b v = v'_{\ell_k+1} + v'_{\ell_k}$ and

$$r_b D_b y_h = (1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}, \quad r_b D_{b \cap \Omega_a} y_h = 2 y'_h|_{T_{k+1}}$$

We have

$$\begin{aligned}
& \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\
&= \varepsilon \left\{ [\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - (1 - \theta_k) \phi'(2 y'_h|_{T_{k+1}}) - \theta_k \phi'(2 y'_h|_{T_k})] v'_{\ell_k} \right. \\
&\quad \left. + [\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) y'_h|_{T_k}) - \phi'(2 y'_h|_{T_k})] v'_{\ell_k} - \theta_k \phi'(y'_h|_{T_k}) v'_{\ell_k+1} \right\}, \quad (\text{A.8})
\end{aligned}$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - |b \cap \Omega_a| r_b \phi(r_b D_{b \cap \Omega_a} y) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) dx \\ &= 2\varepsilon \left(\phi((1 - \theta_k) y'_h|_{T_{k+1}} + (1 + \theta_k) \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi(2 y'_h|_{T_{k+1}}) - (1 + \theta_k) \phi(2 y'_h|_{T_k}) \right). \end{aligned} \quad (\text{A.9})$$

Subcase 3: If $b = (\ell_k \varepsilon, (\ell_k + 2) \varepsilon)$, then $r_b = 2$, $b \cap \Omega_c = (\ell_k \varepsilon, x_k^h)$, $b \cap \Omega_a = (x_k^h, (\ell_k + 2) \varepsilon)$, $r_b D_b v = v'_{\ell_k+2} + v'_{\ell_k+1}$, $D_{b \cap \Omega_a} v = \frac{1}{2 - \theta_k} v'_{\ell_k+2} + \frac{1 - \theta_k}{2 - \theta_k} v'_{\ell_k+1}$, and

$$r_b D_b y_h = y'_h|_{T_{k+2}} + (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} \quad r_b D_{b \cap \Omega_a} y_h = \frac{2}{2 - \theta_k} y'_h|_{T_{k+2}} + \frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}}.$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v dx \\ &= \varepsilon \left\{ \left[\phi'(y'_h|_{T_{k+2}} + (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \phi' \left(\frac{2}{2 - \theta_k} y'_h|_{T_{k+2}} + \frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}} \right) \right] v'_{\ell_k+2} \right. \\ & \quad + \left[\phi'(y'_h|_{T_{k+2}} + (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi' \left(\frac{2}{2 - \theta_k} y'_h|_{T_{k+2}} + \frac{2(1 - \theta_k)}{2 - \theta_k} y'_h|_{T_{k+1}} \right) \right. \\ & \quad \left. \left. - \theta_k \phi'(2 y'_h|_{T_k}) \right] v'_{\ell_k+1} \right\}, \end{aligned} \quad (\text{A.10})$$

Case 2: b is across the *right* atomistic-continuum interface of an atomistic region.

Subcase 1: If $b = (\ell_k \varepsilon, \ell_{k+1} \varepsilon)$, then $r_b = 1$, $b \cap \Omega_c = (x_k^h, (\ell_k + 1) \varepsilon)$, $b \cap \Omega_a = (\ell_k \varepsilon, x_k^h)$, $r_b D_b v = v'_{\ell_k+1}$ and

$$r_b D_b y_h = (1 - \theta_k) y_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}.$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v dx \\ &= \varepsilon \left[\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) - \theta_k \phi'(y'_h|_{T_k}) \right] v'_{\ell_k+1}, \end{aligned} \quad (\text{A.11})$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) dx \\ &= \varepsilon \phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \int_{b \cap T_k} \phi(y'_h|_{T_k}) dx - \int_{b \cap T_{k+1}} \phi(y'_h|_{T_{k+1}}) dx \\ &= \varepsilon \left(\phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) \right). \end{aligned} \quad (\text{A.12})$$

Subcase 2: If $b = (\ell_k \varepsilon, (\ell_k + 2) \varepsilon)$, then $r_b = 2$, $b \cap \Omega_c = (x_k^h, (\ell_k + 2) \varepsilon)$, $b \cap \Omega_a = (\ell_k \varepsilon, x_k^h)$, $r_b D_b v = v'_{\ell_k+2} + v'_{\ell_k+1}$, $r_b D_{b \cap \Omega_a} v = v'_{\ell_k+1}$ and

$$r_b D_b y_h = (2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} \quad \text{and} \quad r_b D_{b \cap \Omega_a} y_h = y'_h|_{T_k}. \quad (\text{A.13})$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v dx \\ &= \varepsilon \left\{ \left[\phi'((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi'(2 y'_h|_{T_k}) - (1 - \theta_k) \phi'(2 y'_h|_{T_{k+1}}) \right] v'_{\ell_k+1} \right. \\ & \quad \left. + \left[\phi'((2 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \phi'(2 y'_h|_{T_{k+1}}) \right] v'_{\ell_k+2} \right\}, \end{aligned} \quad (\text{A.14})$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\ &= \varepsilon \left(\phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k}) - \theta_k \phi(y'_h|_{T_k}) - (1 - \theta_k) \phi(y'_h|_{T_{k+1}}) \right). \end{aligned} \quad (\text{A.15})$$

Subcase 3: If $b = ((\ell_k - 1)\varepsilon, (\ell_k + 1)\varepsilon)$, then $r_b = 2$, $b \cap \Omega_c = (x_k^h, (\ell_k + 1)\varepsilon)$, $b \cap \Omega_a = ((\ell_k - 1)\varepsilon, x_k^h)$, $r_b D_b v = v'_{\ell_{k+1}} + v'_{\ell_k}$, $r_b D_{b \cap \Omega_a} v = \frac{\theta_k}{1 + \theta_k} v'_{\ell_{k+1}} + \frac{1}{1 + \theta_k} v'_{\ell_k}$ and

$$r_b D_b y_h = (1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}} \text{ and } r_b D_{b \cap \Omega_a} y_h = \frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}. \quad (\text{A.16})$$

We have

$$\begin{aligned} & \varepsilon \phi'(r_b D_b y_h) r_b D_b v - |b \cap \Omega_a| \phi'(r_b D_{b \cap \Omega_a} y_h) D_{b \cap \Omega_a} v - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi'(\nabla_{r_b} y_h) \nabla_{r_b} v \, dx \\ &= \varepsilon \left\{ \left[\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) - \phi'(\frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}) \right] v'_{\ell_k} \right. \\ & \quad + \left[\phi'((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) - \theta_k \phi'(\frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}) \right. \\ & \quad \left. \left. - (1 - \theta_k) \phi'(y'_h|_{T_{k+1}}) \right] v'_{\ell_{k+1}}, \right. \end{aligned} \quad (\text{A.17})$$

and

$$\begin{aligned} & \varepsilon \phi(r_b D_b y_h) - \frac{1}{r_b} \int_{b \cap \Omega_c} \phi(\nabla_{r_b} y(x)) \, dx \\ &= 2\varepsilon \left(\phi((1 - \theta_k) y'_h|_{T_{k+1}} + \theta_k y'_h|_{T_k} + y'_h|_{T_{k-1}}) \right. \\ & \quad \left. - (1 + \theta_k) \phi(\frac{2\theta_k}{1 + \theta_k} y'_h|_{T_k} + \frac{2}{1 + \theta_k} y'_h|_{T_{k-1}}) - (1 - \theta_k) \phi(2y'_h|_{T_{k+1}}) \right). \end{aligned} \quad (\text{A.18})$$

APPENDIX B. APPROXIMATION PROPERTIES

In this section, we prove some approximation properties which we have used but are hardly found in standard text books.

Lemma 11. *Let $v \in C^0(\mathbb{R}) \cap W^{1,2}(\mathbb{R})$ be a periodic function with $[a, b]$ being one of its period. Let v_h be a \mathcal{P}_1 interpolation of v with respect to the nodes $a \leq x_0 < x_1 < \dots < x_n \leq b \leq x_{n+1} = x_0 + (b - a)$ in $[x_0, x_{n+1}]$, subject to a constant, i.e., $v_h(x_k) = v(x_k) + C$, for $k = \{1, 2, \dots, n+1\}$, and is extended periodically with period $b - a$. Then the following estimate holds:*

$$\|v'_h\|_{L^2_{[a,b]}} \leq \|v'\|_{L^2_{[a,b]}}, \quad (\text{B.1})$$

where v' and v'_h denote the weak derivatives of v and v_h respectively.

Proof. First we note that, since $v \in C^0(\mathbb{R})$ and v_h is a \mathcal{P}_1 interpolation of v , the weak derivative of v_h on (x_k, x_{k+1}) is defined by

$$v'_h(x) = \frac{v(x_{k+1}) - v(x_k)}{x_{k+1} - x_k}.$$

Since $v \in C^0(\mathbb{R})$ is piecewise differentiable, we have

$$v(x_{k+1}) - v(x_k) = \int_{x_k}^{x_{k+1}} v'(t) \, dt,$$

where v' is the weak derivative of v . By the periodicity of v'_h and v' , and Cauchy-Schwarz Inequality, we have

$$\begin{aligned}
\|v'_h\|_{L^2_{[a,b]}}^2 &= \int_a^b [v'_h(x)]^2 dx \\
&= \int_{x_0}^{x_{n+1}} [v'_h(x)]^2 dx \\
&= \sum_{k=0}^n \int_{x_k}^{x_{k+1}} \left(\frac{v(x_{k+1}) - v(x_k)}{x_{k+1} - x_k} \right)^2 dx \\
&= \sum_{k=0}^n \int_{x_k}^{x_{k+1}} \frac{\left(\int_{x_k}^{x_{k+1}} v'(t) dt \right)^2}{(x_{k+1} - x_k)^2} dx \\
&\leq \sum_{k=0}^n \frac{1}{x_{k+1} - x_k} \left(\int_{x_k}^{x_{k+1}} dt \right) \left(\int_{x_k}^{x_{k+1}} |v'(t)|^2 dt \right) \\
&= \sum_{k=0}^n \int_{x_k}^{x_{k+1}} |v'(t)|^2 dt \\
&= \int_a^b |v'(t)|^2 dt \\
&= \|v'\|_{L^2_{[a,b]}}^2.
\end{aligned}$$

Taking the square root on both sides gives the stated result. \square

Lemma 12. *Let $v \in C^0([a, b]) \cap W^{1,2}([a, b])$ and $I_h v$ is the \mathcal{P}_1 function that interpolates v at the points a and b . We have the following inequality:*

$$\|v' - (I_h v)'\|_{L^2_{(a,b)}}^2 \leq \|v'\|_{L^2_{(a,b)}}^2. \quad (\text{B.2})$$

Proof. Since $v(a) = I_h v(a)$ and $v(b) = I_h v(b)$, by the definition of $I_h v$, we have

$$\int_a^b v' dx = \int_a^b (I_h v)' dx,$$

and equivalently,

$$\int_a^b (v' - (I_h v)') \cdot 1 dx = 0,$$

where v' denotes the weak derivative of v on $[a, b]$. This shows that $(I_h v)'$ is the best L^2 approximation of v' in the space of \mathcal{P}_0 functions as $(I_h v)'$ is a constant. Therefore, by the property of best approximation,

$$\|v' - (I_h v)'\|_{L^2_{(a,b)}}^2 \leq \|v' - C\|_{L^2_{(a,b)}}^2, \quad (\text{B.3})$$

for any constant C . In particular, if we choose C to be 0, the stated result holds. \square

APPENDIX C. DISCRETE SOBOLEV INEQUALITIES ON NON-UNIFORM MESH

In this section, we prove some discrete Sobolev inequalities on non-uniform mesh that are used in the residual analysis for the external force. These results are extensions to the inequalities proved in [7, Lemma A.1, Lemma A.2, Theorem A.4] on non uniform mesh.

Lemma 13. *Let $\mathbf{g} \in \mathbb{R}^L$, $\boldsymbol{\varepsilon}^0, \boldsymbol{\varepsilon}^1 \in \mathbb{R}^L$ and $\varepsilon_i^0, \varepsilon_i^1 > 0 \ \forall i = 1, \dots, L$, $\mathbf{g}' = (g'_i)_{i=2}^L \in \mathbb{R}^{L-1}$, $g'_i := \frac{g_i - g_{i-1}}{\varepsilon_i^1}$ $i = 2, \dots, L$. If $\sum_{i=1}^L \varepsilon_i^0 g_i = 0$, then*

$$|g_i| \leq \frac{1}{h} \sum_{k=2}^L \varepsilon_k^1 |g'_k| \phi_{i,k}, \quad (\text{C.1})$$

where, $h = \sum_{i=1}^L \varepsilon_i^0$, $\phi_{i,k} = \sum_{\ell=1}^{k-1} \varepsilon_\ell^0$ for $k = 2, \dots, i$ and $\phi_{i,k} = \sum_{\ell=k}^L \varepsilon_\ell^0$ for $k = i+1, \dots, L$.

Proof. Let $i \in \{1, \dots, L\}$, then

$$\begin{aligned} h|g_i| &= |hg_i - \sum_{j=1}^L \varepsilon_j^0 g_j| \\ &= \left| \sum_{j=1}^L \varepsilon_j^0 g_i - \sum_{j=1}^L \varepsilon_j^0 g_j \right| \\ &\leq \sum_{j=1}^{i-1} \varepsilon_j^0 |g_i - g_j| + \sum_{j=i+1}^L \varepsilon_j^0 |g_i - g_j|. \end{aligned}$$

Since

$$|g_i - g_j| = \left| \sum_{k=j+1}^i \varepsilon_k^1 g'_k \right|,$$

we have

$$\begin{aligned} h|g_i| &\leq \sum_{j=1}^{i-1} \varepsilon_j^0 \sum_{k=j+1}^i \varepsilon_k^1 |g'_k| + \sum_{j=i+1}^L \varepsilon_j^0 \sum_{k=i+1}^j \varepsilon_k^1 |g'_k| \\ &= \sum_{k=2}^i \varepsilon_k^1 |g'_k| \left(\sum_{j=1}^{k-1} \varepsilon_j^0 \right) + \sum_{k=i+1}^L \varepsilon_k^1 |g'_k| \left(\sum_{j=k}^L \varepsilon_j^0 \right) \\ &= \sum_{k=2}^L \varepsilon_k^1 |g'_k| \phi_{i,k}. \end{aligned}$$

Divide both sides by h , we obtain the stated result. \square

Lemma 14. *(Discrete Poincaré's Inequality) Suppose that $L \geq 1$, $\boldsymbol{\varepsilon}^0, \boldsymbol{\varepsilon}^1 \in \mathbb{R}^L$ with $\varepsilon_i^0, \varepsilon_i^1 > 0$, $\forall i = 1, \dots, L$. Let $\mathbf{g} \in \mathbb{R}^L$ such that $\sum_{i=1}^L \varepsilon_i^0 g_i = 0$ and $\mathbf{g}' = (g'_i)_{i=2}^L \in \mathbb{R}^{L-1}$ such that $g'_i = \frac{g_i - g_{i-1}}{\varepsilon_i^1}$. Define \mathcal{D}_0 to be the set $\{1, \dots, L\}$ and \mathcal{D}_1 to be the set $\{2, \dots, L\}$, then*

$$\|\mathbf{g}\|_{\ell^p_{\boldsymbol{\varepsilon}^0(\mathcal{D}_0)}} \leq \frac{1}{2} \frac{L^2 \max\{\max_{1 \leq i \leq L} \varepsilon_i^0, \max_{2 \leq k \leq L} \varepsilon_k^1\}^2}{h} \|\mathbf{g}'\|_{\ell^p_{\boldsymbol{\varepsilon}^1(\mathcal{D}_1)}}, \quad (\text{C.2})$$

for $p \in \{1, \infty\}$, where $h = \sum_{i=1}^L \varepsilon_i^0$.

Proof. Using the result of Lemma 13, we have

$$\begin{aligned} \sum_{i=1}^L \varepsilon_i^0 |g_i| &\leq \sum_{i=1}^L \frac{\varepsilon_i^0}{h} \sum_{k=2}^i \varepsilon_k^1 |g'_k| \phi_{i,k} + \sum_{i=1}^L \frac{\varepsilon_i^0}{h} \sum_{k=i+1}^L \varepsilon_k^1 |g'_k| \phi_{i,k} \\ &= \frac{1}{h} \left[\sum_{k=2}^L \left(\sum_{i=1}^L \varepsilon_i^0 \phi_{i,k} \right) \varepsilon_k^1 |g'_k| \right]. \end{aligned}$$

Since

$$\sum_{i=1}^L \varepsilon_i^0 \phi_{i,k} \leq \max_{1 \leq i \leq L} \varepsilon_i^0 \sum_{i=1}^L \phi_{i,k} = \max_{1 \leq i \leq L} \varepsilon_i^0 \left[\sum_{i=1}^{k-1} \phi_{i,k} + \sum_{i=k}^L \phi_{i,k} \right],$$

and

$$\begin{aligned} \sum_{i=1}^{k-1} \phi_{i,k} + \sum_{i=k}^L \phi_{i,k} &\leq (k-1) \sum_{\ell=k}^L \varepsilon_\ell^0 + (L - (k-1)) \sum_{\ell=1}^{k-1} \varepsilon_\ell^0 \\ &\leq [(k-1)(L - (k-1)) + (L - (k-1))(k-1)] \max_{1 \leq i \leq L} \varepsilon_i^0 \\ &\leq \frac{1}{2} \max_{1 \leq i \leq L} \varepsilon_i^0 L^2. \end{aligned}$$

Put these results together, we obtain the stated result for $p = 1$. For $p = \infty$,

$$\begin{aligned} |g_i| &\leq \frac{1}{h} \sum_{k=2}^L \varepsilon_k^1 |g'_k| \phi_{i,k} \\ &\leq \frac{1}{h} \left[\sum_{k=2}^i \varepsilon_k^1 |g'_k| \phi_{i,k} + \sum_{k=i+1}^L \varepsilon_k^1 |g'_k| \phi_{i,k} \right] \\ &\leq \frac{1}{h} \sum_{k=2}^L \phi_{i,k} \max_{2 \leq k \leq L} \varepsilon_k^1 |g'_k| \\ &\leq \frac{1}{2} \frac{L^2 \max_{1 \leq i \leq L} \varepsilon_i^0}{h} \max_{2 \leq k \leq L} \varepsilon_k^1 |g'_k|. \end{aligned}$$

The stated result is obtained by taking the maximum of ε_i^0 and ε_k^1 over \mathcal{D}_0 and \mathcal{D}_1 . \square

Lemma 15. (*Discrete Friedrichs' Inequality*) Suppose that $L \geq 1$, ε^0 , ε^1 , \mathcal{D}_0 , \mathcal{D}_2 are the same as in Lemma 14. Let $\mathbf{f} \in \mathbb{R}^L$ such that $f_1 = f_L = 0$, and $\mathbf{f}' = (f'_i)_{i=2}^L \in \mathbb{R}^{L-1}$ such that $f'_i = \frac{f_i - f_{i-1}}{\varepsilon_i^1}$, then

$$\|\mathbf{f}\|_{\ell^p_{\varepsilon^0(\mathcal{D}_0)}} \leq \frac{1}{2}(L-1) \max_{2 \leq i \leq L-1} \max\{\varepsilon_i^0, \varepsilon_i^1\} \|\mathbf{f}'\|_{\ell^p_{\varepsilon^1(\mathcal{D}_1)}}, \quad (\text{C.3})$$

for $p \in \{1, \infty\}$.

Proof. For $p = 1$,

$$\begin{aligned}
\sum_{i=1}^L \varepsilon_i^0 |f_i| &= \sum_{i=2}^{L-1} \varepsilon_i^0 |f_i| \\
&= \frac{1}{2} \sum_{i=2}^{L-1} \varepsilon_i^0 \left[\left| \sum_{j=2}^i (f_j - f_{j-1}) \right| + \left| \sum_{j=i+1}^L (f_j - f_{j-1}) \right| \right] \\
&\leq \frac{1}{2} \sum_{i=2}^{L-1} \varepsilon_i^0 \left[\sum_{j=2}^i \varepsilon_j^1 |f'_j| + \sum_{j=i+1}^L \varepsilon_j^1 |f'_j| \right] \\
&= \frac{1}{2} \sum_{i=2}^{L-1} \varepsilon_i^0 \sum_{j=1}^L \varepsilon_j^1 |f'_j| \\
&\leq \frac{1}{2} (L-1) \max_{2 \leq i \leq L-1} \varepsilon_i^0 \sum_{j=1}^L \varepsilon_j^1 |f'_j|.
\end{aligned}$$

For $p = \infty$,

$$|f_i| \leq \sum_{j=2}^i \varepsilon_j^1 |f'_j| = (i-1) \max_{2 \leq j \leq L} \varepsilon_j^1 \max_{2 \leq j \leq L} |f'_j|,$$

and

$$|f_i| \leq \sum_{j=i+1}^L \varepsilon_j^1 |f'_j| = (L-i) \max_{2 \leq j \leq L} \varepsilon_j^1 \max_{2 \leq j \leq L} |f'_j|.$$

Thus we have

$$\begin{aligned}
\max_{i \in \mathcal{D}_0} |f_i| &\leq \min(i-1, L-i) \max_{2 \leq j \leq L} \varepsilon_j^1 \max_{2 \leq j \leq L} |f'_j| \\
&\leq \frac{1}{2} (L-1) \max_{2 \leq j \leq L} \varepsilon_j^1 \max_{2 \leq j \leq L} |f'_j|.
\end{aligned}$$

□

Remark 2. The bounds we have got here are not optimal as if ε_i 's and $\bar{\varepsilon}_j$'s vary too much, taking the maximum of them in the inequalities could significantly reduce the sharpness of the estimate. However, for the analysis of this paper, such a bound is optimal enough to produce efficient error estimators and we leave the work of looking for optimal bounds to future work. □

Theorem 16. (bounds on the interpolation error) Let $L \geq 1$, $\varepsilon^0, \varepsilon^1, \varepsilon^2 \in \mathbb{R}^L$, with $\varepsilon_i^0, \varepsilon_i^1, \varepsilon_i^2 > 0 \forall i = 1, \dots, L$. Let $\mathbf{f} \in \mathbb{R}^L$ and $\mathbf{F} \in \mathbb{R}^L$ such that $F_1 = f_1$ and

$$F_i = f_1 + \frac{\sum_{j=2}^i \varepsilon_j^0}{h} (f_L - f_1) \quad i = 2, \dots, L, \quad (\text{C.4})$$

where $h = \sum_{i=2}^L \varepsilon_i^0$. Define $\mathbf{f}' = (f'_i)_{i=2}^L \in \mathbb{R}^{L-1}$ such that $f'_i = \frac{f_i - f_{i-1}}{\varepsilon_i^1}$ and $\mathbf{f}'' = (f''_i)_{i=2}^{L-1} \in \mathbb{R}^{L-2}$ such that $f''_i = \frac{f'_{i+1} - f'_i}{\varepsilon_i^2}$, and \mathbf{F}' and \mathbf{F}'' are defined in the same way. Let $\mathcal{D}_0, \mathcal{D}_1$ be the same sets defined in Lemma 14 and \mathcal{D}_2 be the set $\{2, \dots, L-1\}$. Then, for $p \in \{1, \infty\}$,

$$\|\mathbf{f} - \mathbf{F}\|_{\ell^p_{\varepsilon^0}(\mathcal{D}_0)} \leq \frac{1}{4} \frac{L^3 \max_{2 \leq i \leq L-1} \varepsilon_i^0 \max_{2 \leq j \leq L-1} \varepsilon_j^1 \max_{2 \leq k \leq L-1} \varepsilon_j^2}{h} \|\mathbf{f}''\|_{\ell^p_{\varepsilon^2}(\mathcal{D}_2)}. \quad (\text{C.5})$$

Proof. Let $\mathbf{g} = \mathbf{f} - \mathbf{F}$, by the definition of \mathbf{F} , we have $g_1 = g_L = 0$ and

$$\sum_{i=2}^L \varepsilon_i g'_i = \sum_{i=2}^L (f_i - f_{i-1}) - \sum_{i=2}^L (F_i - F_{i-1}) = 0.$$

By Lemma 15,

$$\|\mathbf{g}\|_{\ell_{\varepsilon}^p(\mathcal{D}_0)} \leq \frac{1}{2}(L-1) \max_{2 \leq i \leq L-1} \max\{\varepsilon_i^0, \varepsilon_i^1\} \|\mathbf{g}'\|_{\ell_{\varepsilon}^p(\mathcal{D}_1)},$$

as $g_1 = g_L = 0$, and by Lemma 14,

$$\|\mathbf{g}'\|_{\ell_{\varepsilon}^p(\mathcal{D}_1)} \leq \frac{1}{2} \frac{L^2 \max\{\max_{1 \leq i \leq L} \varepsilon_i^1, \max_{2 \leq k \leq L-1} \varepsilon_k^2\}^2}{h} \|\mathbf{g}''\|_{\ell_{\varepsilon}^p(\mathcal{D}_2)},$$

as $\sum_{i=2}^L \varepsilon_i g'_i = 0$. Since $\mathbf{F}'' = 0$, from which we know $\mathbf{g}'' = \mathbf{f}''$, the stated estimate holds. \square

REFERENCES

- [1] Marcel Arndt and Mitchell Luskin. Goal-oriented atomistic-continuum adaptivity for the quasicontinuum approximation. *Int. J. Multiscale Comput. Engrg.*, 5(49-50):407–415, 2007.
- [2] Marcel Arndt and Mitchell Luskin. Error estimation and atomistic-continuum adaptivity for the quasicontinuum approximation of a Frenkel-Kontorova model. *Multiscale Model. Simul.*, 7(1):147–170, 2008.
- [3] Marcel Arndt and Mitchell Luskin. Goal-oriented adaptive mesh refinement for the quasicontinuum approximation of a Frenkel-Kontorova model. *Comput. Methods Appl. Mech. Engrg.*, 197(49-50):4298–4306, 2008.
- [4] W. E and P. Ming. Analysis of the local quasicontinuum method. In *Frontiers and prospects of contemporary applied mathematics*, volume 6 of *Ser. Contemp. Appl. Math. CAM*, pages 18–32. Higher Ed. Press, Beijing, 2005.
- [5] P. Lin. Theoretical and numerical analysis for the quasi-continuum approximation of a material particle model. *Math. Comp.*, 72(242):657–675, 2003.
- [6] C. Ortner and A.V. Shapeev. A priori error analysis of an energy-based atomistic/continuum coupling method for pair interactions in two dimensions. arXiv:1104.0311v1.
- [7] C. Ortner and E. Süli. Analysis of a quasicontinuum method in one dimension. *M2AN Math. Model. Numer. Anal.*, 42(1):57–91, 2008.
- [8] C. Ortner and H. WANG. A priori error estimates for energy-based quasicontinuum approximations of a periodic chain. 2010. to appear in M3AS Math. Model. Meth. Appl. Sci.
- [9] Serge Prudhomme, Paul. Bauman, and Tinsley Oden. Error control for molecular statics problems. *Int. J. Multiscale Comput. Engrg.*, 4:647–662, 2007.
- [10] A.V. Shapeev. Consistent energy-based coupling of atomistic and continuum static models for two-body potential. arXiv:1010.0512.
- [11] T. Shimokawa, J.J. Mortensen, J. Schiotz, and K.W. Jacobsen. Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region. *Phys. Rev. B*, 69(21):214104, 2004.

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